CHEMCAD Version 6

User Guide

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CHEMCAD Version 6 User Guide

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Chapter 1

Introduction to CHEMCAD

Welcome to CHEMCAD Version 6.0, a powerful and effective software tool for chemical process simulation. Whether you're a new or experienced CHEMCAD user, you'll appreciate the program's user-friendly, feature-rich interface. Creating flowsheets and running simulations is fast and easy with CHEMCAD, and the program is highly customizable to fit your needs and the way you work.

This manual will help you get up and running with CHEMCAD, from installation and licensing to tutorials that walk you through real-world examples.

Overview of CHEMCAD and Its Uses

Today's chemical processing industry (CPI) faces numerous challenges: rising fuel and feedstock costs, reduced engineering staff, shorter product life cycles, increased global competition, and increased regulation. These challenges require that CPI companies seek out and use the best tools to increase productivity and improve engineering decisions.

CHEMCAD is a powerful and flexible chemical process simulation environment, built around three key values of innovation, integration, and open architecture. These values create important advantages for CHEMCAD users:

- The latest chemical engineering techniques at your fingertips
- All functionality united in a single software environment
- Seamless connection to the chemical engineering computing environment, with links to tools such as MS Excel and Word and interfaces such as COM, DCOM, OPC, CAPE-OPEN, and XML

CHEMCAD combines a state-of-the-art graphical user interface (GUI), an extensive chemical component database, a large library of thermodynamic data, and a library of the most common unit operations to give users the ability to provide significant and measurable returns on their investment. In addition, the program is customizable to allow custom chemicals, thermodynamics, unit operations, calculations, and reporting—all ingredients for a powerful user experience.

CHEMCAD is capable of modeling continuous, batch, and semi-batch processes, and it can simulate both steady-state and dynamic systems. This program is used extensively around the world for the design, operation, and maintenance of chemical processes in a wide variety of industries, including oil and gas exploration, production, and refining; gas processing; commodity and specialty chemicals; pharmaceuticals; biofuels; and process equipment manufacturing.

Within all of these industries, chemical engineers work every day with CHEMCAD to address a variety of challenges:

- Initial design of new processes
- Optimization or de-bottlenecking of existing processes
- Performance monitoring of processes
- Design and rating of process equipment such as vessels, columns, heat exchangers, piping, valves, and instrumentation
- Evaluation of safety relief devices
- Heat exchanger sizing
- Pressure and flow balancing of complex piping networks
- Reconciliation of plant data
- Economic comparisons of process alternatives
- Advanced process control (APC), including model predictive control (MPC), real-time optimization (RTO), and operator training systems (OTS)
- Scale-up of processes from lab-scale to pilot-scale, and from pilot-scale to full-scale
- Binary interaction parameter (BIP) regression from process or lab data
- Batch reaction rate regression from process or lab data

No matter how complex your process, CHEMCAD is capable of delivering the results you need to stay competitive in an increasingly fast and fluid global market. Easy to learn and highly customizable, CHEMCAD can put future-proof solutions within easy reach of your engineering staff.

CHEMCAD Products and Features

The CHEMCAD suite consists of several modules that serve specific purposes. Depending on your particular needs, you may have purchased some or all of these modules. The following are brief descriptions of the various CHEMCAD modules and their most common uses.

CC-STEADY STATE

The main CHEMCAD product, known as CC-STEADY STATE, enables you to design new processes, rate existing processes, and optimize processes in steady state.

CC-DYNAMICS

The module known as CC-DYNAMICS makes it possible to design and rate existing processes using a dynamic simulation. This module is fully integrated with CHEMCAD to make switching between steady state and dynamics easy and intuitive. Using CC-DYNAMICS, you can easily simulate everything from simple vessel accumulation to complex control systems on columns. This module also provides tools for simulation of continuous stirred-tank reactors (CSTRs), including complex reaction rate and pressure calculation.

CC-BATCH

The CC-BATCH product enables you to design, rate, or optimize a batch distillation column. CC-BATCH includes a scheduling interface to allow an "operation step" approach to simulation of batch columns.

CC-THERM

The CC-THERM product lets you design a single heat exchanger, or vet a vendor's heat exchanger design. It is also ideal for customers who want to rate existing exchangers in new service, or to perform calculations on hypothetical situations. CC-THERM can simulate shell-and-tube, air-cooled, plate-and-frame, and double-pipe exchangers. Full integration with CHEMCAD makes it possible to calculate exit conditions from exchanger geometry for high-fidelity simulations.

CC-SAFETY NET

The CC-SAFETY NET product provides the capability to design or rate piping networks and safety relief devices and systems, in both steady-state and dynamic systems. The steady-state features of CC-SAFETY NET are included with CC-STEADY STATE. This product enables users to make simultaneous flow- and pressure-balanced simulations—even in reverse-flow situations—for single- or multi-phase flow.

CC-FLASH

The CC-FLASH module provides physical property and phase equilibrium data, as well as property prediction and regression. CC-FLASH is a subset of CC-STEADY STATE, and is meant for customers who do not need full flowsheet simulation tools.

CHEMCAD Features by Module

The following matrix lists the features associated with each component of the CHEMCAD suite. For a more detailed explanation, or to inquire about a particular component or feature, please contact Chemstations or your CHEMCAD distributor (see complete contact information at www.chemstations.net/contact.htm).

	CC-STEADY STATE	CC-DYNAMICS	CC-BATCH	CC-THERM	CC-SAFETY NET	CC-FLASH
VB/COM/OPC/Data Map	✓	✓				
Sensitivity/optimization	✓	✓			✓	
Sizing (line/valve/orifice/vessel)	✓	✓			✓	
Run steady state	✓		✓	✓	✓	✓
Run dynamics		✓			✓	
Run recycles	✓	✓			✓	
Costing	✓	✓			✓	
Reconciliation	✓	✓				
Sizing columns	✓	✓	✓			
Sizing heat exchangers				✓		
Economics	✓	✓				
Reports (incl. Excel)	✓	✓	✓	✓	✓	✓
DIERS	✓	✓			✓	
CO_2 solid	✓	✓			✓	✓
Hydrates	✓	✓			✓	✓
Depress	✓	✓			✓	✓
TOC/COD	✓	✓			✓	✓
Pure regression	✓	✓	✓	✓	✓	✓
BIP regression	✓	✓	✓	✓	✓	✓
Electrolyte regression	✓	✓	✓	✓	✓	✓
Rate regression	✓	✓				
Units calculator	✓	✓	✓	✓	✓	✓
Execute parser	✓	✓				
Environmental report	✓	✓	✓	✓	✓	✓
Simple calculator	✓	✓	✓	✓	✓	✓
Spec sheet	✓	✓	✓	✓	✓	

UnitOps by Module

The availability of certain unit operations, or UnitOps, in CHEMCAD simulations is a function of which modules you have licensed. The following matrix lists all available UnitOps and the CHEMCAD modules associated with them.

	CC-STEADY STATE	CC-DYNAMICS	CC-BATCH	CC-THERM	CC-SAFETY NET	CC-FLASH
Baghouse filter	✓	✓				
Batch column			✓			
Batch reactor		✓				
Calculator	✓	✓				
Centrifuge	✓	✓				
Component separator	✓	✓				
Compressor	✓	✓			✓	
Control valve	✓	✓			✓	
Controller	✓	✓			✓	
Crusher/grinder	✓	✓				
Crystallizer	✓	✓				
Cyclone	✓	✓				
Divider	✓	✓			✓	✓
Dynamic vessel		✓			✓	
Electrostatic precipitator	✓	✓				
Equilibrium reactor	✓	✓				
Excel unit	✓	✓				
Expander	✓	✓			✓	
Fired heater	✓	✓				
Flash	✓	✓			✓	✓
Gibbs reactor	✓	✓				
Heat exchanger	✓	✓		✓	✓	
Hydrocyclone	✓	✓				
Kinetic reactor	✓	✓				
Liquid/liquid extractor	✓	✓				
LLV flash*	✓	✓				
LNGH exchanger	✓	✓				

	CC-STEADY STATE	CC-DYNAMICS	CC-BATCH	CC-THERM	CC-SAFETY NET	CC-FLASH
Loop	✓	✓				
Mixer	✓	✓			✓	✓
Node	✓	✓			✓	
Phase generator*	✓	✓				
PID controller	✓	✓			✓	
Pipe simulator	✓	✓			✓	
Polymer reactor						
Pump	✓	✓			✓	
Ramp controller	✓	✓			✓	
Recorder*	✓					
Run subflowsheet META unit	✓	✓				
SCDS distillation column	✓	✓				
Screen	✓	✓				
Sedimentator	✓	✓				
Shortcut column	✓	✓				
Solids dryer	✓	✓				
Solids washer	✓	✓				
Stoichiometric reactor	✓	✓				
Stream reference	✓	✓				
Tank			✓			
Time delay		✓			✓	
Time switch		✓	✓			
Tower distillation column	✓	✓				
Tower plus distillation column	✓	✓				
User-added module	✓	✓				
Vacuum filter	✓	✓				
Valve	✓	✓			✓	
Venturi scrubber	✓	✓				
Vessel*	✓	✓				

*** These UnitOps will be phased out eventually.**

Chapter 2

Getting Started with CHEMCAD

Now that you have CHEMCAD in hand, you probably want to get started right away. Let's get directly to the point, with step-by-step instructions for installing and licensing the program.

Installing the Software

Start by ensuring that your PC meets the minimum system requirements, as listed below. It's also a good idea to find out before you begin whether your copy of CHEMCAD will rely on a network license; if it will, make sure to ask your network administrator for all the information that you'll need when installation is complete and it's time to set up licensing.

CHEMCAD System Requirements

Processor speed: 500 MHz or higher

Operating system: Windows 2000, XP, or Vista

RAM: 256 MB

Video card: 128 MB or higher video memory

Display resolution: 1024 x 768 or higher

Hard disk space: 500 MB (750 MB during installation)

Productivity software: Some features require Microsoft Office®

Once you've established that your computer is ready for installation, insert the CHEMCAD 6.0 disc into an available CD media drive and watch for the CHEMCAD splash screen to appear.

Note: If you insert the disc and close the CD media drive door, but nothing happens within one minute, then your system is not configured to launch the CD content automatically. To launch the installation program manually, go to My Computer, double-click the icon for your computer's CD media drive, and then double-click the file called **Setup.exe**.

Click **Install CHEMCAD** to launch the InstallShield Wizard. InstallShield inspects your computer for software components that CHEMCAD will need, and prompts you to install any needed components with a screen similar to Figure 2-01.

InstallShield Wizard
CHEMCAD Suite requires that the following requirements be installed on your computer prior to installing this application. Click OK to begin installing these requirements:
Status
Requirement
Pending
Microsoft XML Core Services 6.0
Pending
Microsoft Visual Studio 2005 Tools for Applications
Install
Cancel

Figure 2-01: InstallShield Wizard screen listing software components to be installed

Click **Install** to continue. Follow the prompts on all other screens until you see the CHEMCAD Suite – InstallShield Wizard screen, shown in Figure 2-02.

Note: Depending on how many software components InstallShield identifies, there may be quite a few screens, and the procedure could take several minutes. Once these components are installed on your computer, however, you will *not* need to reinstall them with future CHEMCAD updates.

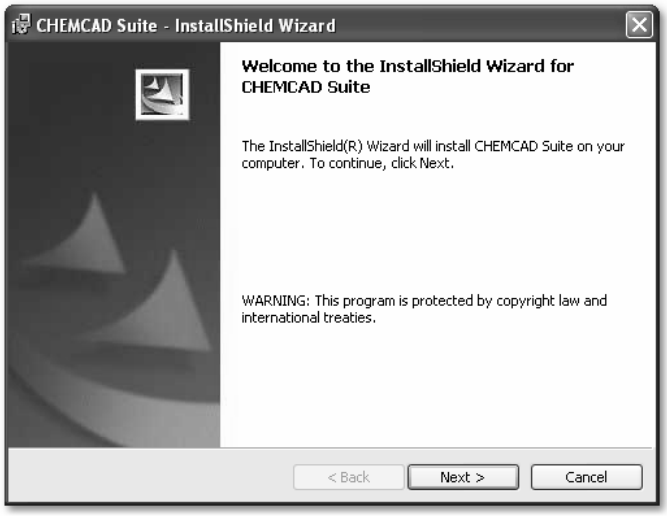
CHEMCAD Suite - InstallShield Wizard
Welcome to the InstallShield Wizard for CHEMCAD Suite
The InstallShield(R) Wizard will install CHEMCAD Suite on your computer. To continue, click Next.
WARNING: This program is protected by copyright law and international treaties.
< Back
Next >
Cancel

Figure 2-02: The CHEMCAD Suite - InstallShield Wizard screen

Click **Next** to begin the installation process. The License Agreement screen appears, listing the CHEMCAD standard license. Once you've read and understood the terms of the license, you'll need to click the *I accept the terms of the license agreement* button before you can click **Next** again to proceed. Note that you have the option to print a copy of the license agreement from this screen.

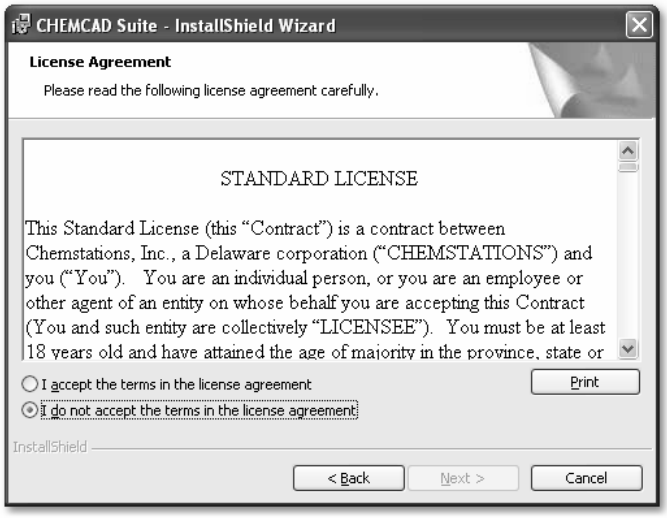
CHEMCAD Suite - InstallShield Wizard
License Agreement
Please read the following license agreement carefully.
STANDARD LICENSE
This Standard License (this "Contract") is a contract between Chemstations, Inc., a Delaware corporation ("CHEMSTATIONS") and you ("You"). You are an individual person, or you are an employee or other agent of an entity on whose behalf you are accepting this Contract (You and such entity are collectively "LICENSEE"). You must be at least 18 years old and have attained the age of majority in the province, state or
I accept the terms in the license agreement
I do not accept the terms in the license agreement
Print
InstallShield
< Back
Next >
Cancel

Figure 2-03: The Standard License screen

The Destination Folder screen appears next, displaying the name of the folder into which the CHEMCAD files will be installed by default. Normally, this destination is **C:\Program Files\Chemstations\CHEMCAD**, and it is recommended that you use this location unless you have a specific need to install the program elsewhere. Click the **Change** button if you want to change the file destination, or click **Next** to accept the suggested destination and proceed.

The Setup Type screen now appears, offering a choice between complete and custom installation. Each type of installation is described on the screen. Either accept the default setting of **Complete** or click **Custom** to select specific components to install, then click **Next** to proceed.

The Ready to Install the Program screen now appears. Note that on this screen, and in fact on any screen in the installation process, you can click **Back** to return to a previous screen and verify or change your installation settings. If you are satisfied with your settings as they are, click **Next** to start the installation.

The Installing CHEMCAD Suite screen appears, showing the progress of your installation with a green status bar.

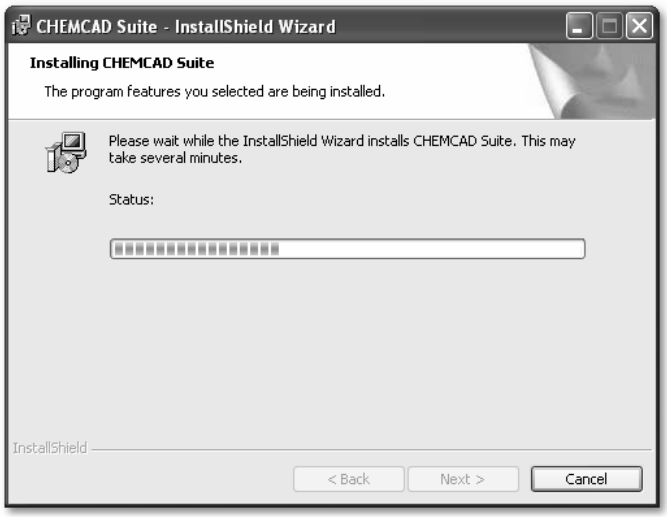
CHEMCAD Suite - InstallShield Wizard
Installing CHEMCAD Suite
The program features you selected are being installed.
Please wait while the InstallShield Wizard installs CHEMCAD Suite. This may take several minutes.
Status:
InstallShield
< Back
Next >
Cancel

Figure 2-04: Status bar showing the progress of CHEMCAD installation

When installation is complete, you'll see one final screen, which states that the InstallShield Wizard has completed installation of the CHEMCAD Suite. Click **Finish** to close the installation program and open CHEMCAD 6.

Licensing CHEMCAD

Before you can use CHEMCAD, you'll need to set up a licensing scheme of some type. Depending on your particular licensing agreement, you will use one of several types of licenses to run CHEMCAD.

Types of CHEMCAD Licenses

The various types of CHEMCAD licenses are designed to fit different users' software, hardware, and networking needs. Most licenses require the use of a hardware device, commonly known as a *dongle*, to run the program.

The dongle simply plugs into either a USB port or a parallel port on the computer, and must be plugged in any time the program runs. If you work on a network with other CHEMCAD users, your license may rely on a dongle plugged into a network server elsewhere in your organization, rather than one plugged directly into your computer.

You or your organization will use one of four types of dongles:

- SuperPro single-user dongle (parallel or USB connection)
- SuperPro Net dongle (parallel or USB connection)
- Sentinel Scribe single-user dongle (parallel connection)
- NetSentinel network dongle (parallel connection)

In some instances, software licensing is accomplished without the use of a hardware device:

- License Manager software, which runs over a local- or wide-access network
- System Authorization, a method that authorizes a single-user machine for a limited time (used for software evaluation)

License Settings

To run CHEMCAD for the first time, make sure that your dongle (if applicable) is plugged in properly, and then start the program. From the Windows Start menu, select **All Programs** > **Chemstations** > **CHEMCAD**.

The program opens, displaying a CHEMCAD splash screen. After a few moments, that screen is replaced by the License Settings screen.

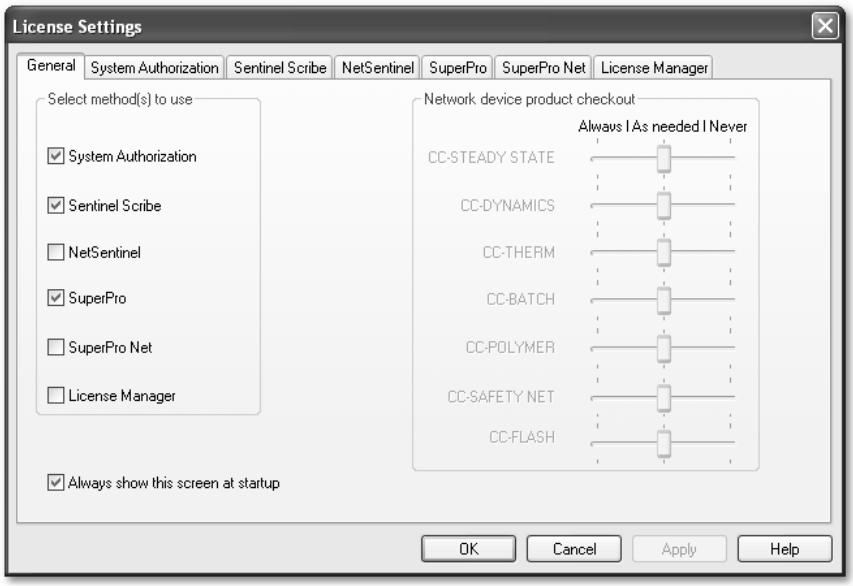

Figure 2-05: The License Settings screen with default settings

The checked boxes on the left side of this screen indicate the types of licensing hardware and software that CHEMCAD will search for when you click **OK**. Note that network licensing methods are not checked; this saves time for many users, because searching for a network dongle can be time-consuming.

Note: If you are using one of the network licensing methods (NetSentinel, SuperPro Net, or License Manager), you'll need to check the appropriate box before clicking **OK**. You can also click the other boxes to clear their check marks and speed up CHEMCAD's search for your license.

On the right side of the screen, the *Network device product checkout* area lets network users choose whether or not to request licenses for specific CHEMCAD modules. For each listed product, you can elect to secure a license **Always**, **As needed**, or **Never**.

The default setting for all of these slider controls is **As needed**, which secures a license only when you begin to use a specific CHEMCAD feature controlled by a certain product. This setting is ideal in most situations, as it leaves unneeded licenses available for other users. To change any module's checkout setting, simply click to the left or right of the current setting to move the slider.

In most cases, you won't need to make any changes on the License Settings screen, although you may want to clear the *Always show this screen at startup* check box, to avoid seeing this screen each time you start CHEMCAD.

Note: If you've turned off this check box, you can still open the License Settings dialog box at any time. Either select **Tools** > **Options** > **License Settings** from within an open simulation, or select **License** > **License Settings** with no simulation open.

When you've made any changes needed, click **OK**. Once CHEMCAD has located your valid license, you'll see the Licenses in Use screen, which lists all licensed products along with the type of license device or software validating each product. Click **OK** to close this screen and access the main CHEMCAD window.

Updating a License

CHEMCAD dongles require re-programming on a regular basis, either once a year or more often depending on your licensing agreement. This is a security measure to reduce the likelihood that your dongle will be stolen and misused.

The dongle that you use is programmed to work only through the licensed time period, and when that time has elapsed, the dongle must be updated before you can continue using CHEMCAD.

Updating a dongle is a relatively simple procedure. Before your license expiration, you or your software administrator should receive an e-mail from Chemstations, with what's known as a *configuration file* included as an attachment. You should save this file to your Windows desktop as soon as you receive it.

Note: If you've updated the same dongle in the past, the new configuration file should have the exact same file name as the previous one. If, while saving the file to your desktop, you see a Windows message about an existing file with the same name, you should overwrite the old file (which in any case cannot be used again), replacing it with the new one.

It's important to ensure that your configuration file matches your dongle. The configuration file should be a .DNG file whose name includes a four- or five-digit code; this code must match the number stamped onto your dongle. If the numbers don't match, contact your software administrator or Chemstations support to resolve the issue.

The update e-mail also specifies the date on which you'll need to update your dongle. Before that date arrives, follow this procedure to perform the update:

1. Start the CHEMCAD program; you should see the License Settings dialog box appear automatically. If necessary, you can open this dialog box using either **Tools** > **Options** > **License Settings** (with a simulation open) or **License** > **License Settings** (with no simulation open).
2. Within the License Settings dialog box, click the tab with the same name as the type of hardware dongle that you use: **Sentinel Scribe**, **NetSentinel**, **SuperPro**, or **SuperPro Net**.
3. On the tab you've selected, find the **Re-program** button—**Re-program SentinelSuperPro**, for example. Click this button to begin the re-programming procedure.

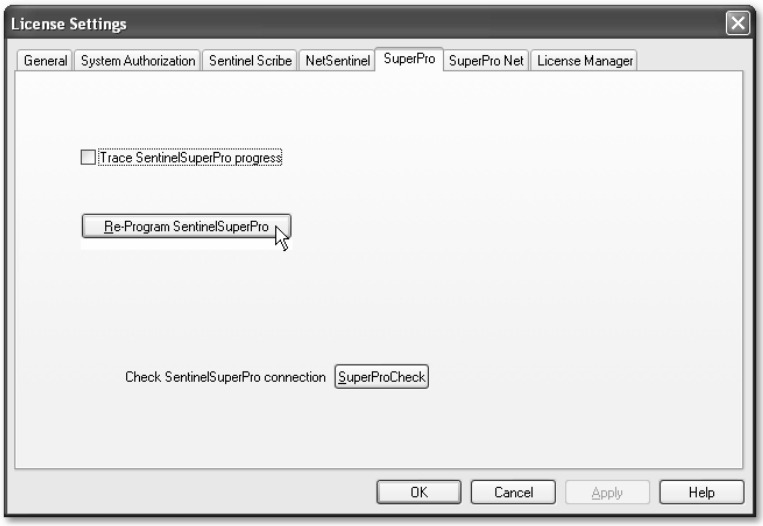

Figure 2-06: Re-programming a SuperPro dongle from the License Settings dialog box

4. When the Browse for Folder dialog box appears, navigate to the location where you saved the .DNG configuration file. Normally, this is the Windows desktop; if you saved your configuration file there, click **Desktop** to tell CHEMCAD where to look for the file, then click **OK**.

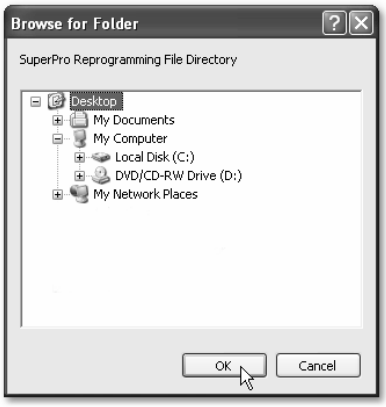

Figure 2-07: Selecting the location where the configuration file resides

5. CHEMCAD re-programs the dongle and then displays a "success" pop-up window.

Figure 2-08: Successful re-programming of a CHEMCAD dongle

6. Click **OK** to close the pop-up window. If the Licenses in Use screen appears, click **OK** to close it.

You should now be able to open CHEMCAD and proceed normally.

Getting Help with CHEMCAD

If you find that you have questions that are not addressed in this User Guide, you can turn to several resources for CHEMCAD help.

Online Help

At any time while running CHEMCAD in an active window, you can press the **[F1]** key to bring up the CHEMCAD Help screen that's most appropriate to the task you are currently performing or the dialog box currently displayed.

In some situations, pressing **[F1]** will bring up the main CHEMCAD 6 Help window instead of a particular help screen. From there, you can click the **Contents**, **Index**, or **Search** tab in the upper left corner of the CHEMCAD 6 Help window, and use these tools to find the information you need.

You can also go directly to the main CHEMCAD 6 Help window by selecting **Help** > **Help Topics** from the CHEMCAD main menu. Regardless of how you open CHEMCAD Help, it always opens in a separate window that does not interfere with the operation of the CHEMCAD program.

CHEMCAD Coach

The CHEMCAD Coach pane is a tool that you can open within CHEMCAD to view concise instructions for common procedures. To see a list of available topics, select **Help** > **CHEMCAD Coach**. Then click on any link in the CHEMCAD Coach window to view the instructions for a specific task.

Procedure Demos

Animated demonstrations of common tasks are available to help you get started using the CHEMCAD program. Topics covered include the various steps involved in creating a basic simulation; procedures for simulations involving batch reactors, heat exchanger sizing, and piping; control valve rating and sizing; creating an Excel Data Map; and updating a licensing dongle.

The demo files are installed along with CHEMCAD. To access these demos, select **Start** > **All Programs** > **Chemstations** > **Demos**, and then browse the list of available topics. Click the button for the demo you'd like to view and then click **Play** to run the demo.

The Chemstations Web Site

To find the most recent updates of the CHEMCAD software, manuals, and various training tools, go to www.chemstations.net. There you'll find the following items available for download:

- The latest release of CHEMCAD
- A list of updates implemented in the most recent release
- The latest version of CHEMCAD 6.0 Help
- CHEMCAD 6.0 Interactive Demos
- Programming guides for interfacing with CHEMCAD

Contacting Chemstations Technical Support

If you are unable to solve a problem or find the answer to a question using this manual or the other tools listed here, you can contact Chemstations' technical support staff for assistance.

Our technical support engineers are available via e-mail, or by phone Monday through Friday, 7:00 AM through 6:00 PM Central Standard Time.

Phone:	713.978.7700
Toll-free (U.S. and Canada):	800.243.6223
FAX:	713.978.7727
E-mail:	support@chemstations.com

Outside of the United States, please see www.chemstations.com for regional contact information.

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Chapter 3

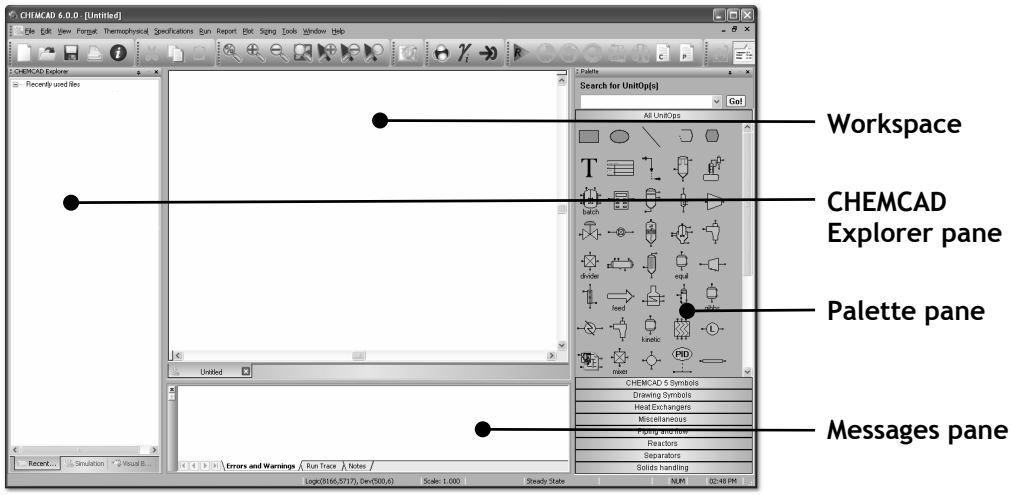
The CHEMCAD Interface

With the release of Version 6.0, the CHEMCAD interface has undergone quite a transformation. For this reason, even long-time users of CHEMCAD will benefit from a review of the program's screen layout and the location of important features.

This chapter takes you on a tour of the CHEMCAD screen, including the menus and toolbars, the main areas of the screen, and the flowsheet drawing tools. It also shows you some ways that you can customize the screen layout so that it best suits your own way of working.

The CHEMCAD Window

When you launch the CHEMCAD program for the first time, you'll see a screen with a large white area in the middle and various *panes*, or specialized areas, at the edges of the screen.



The Workspace

The area in the middle of the screen is known as the *workspace*. This is the main focus of the CHEMCAD window, the place where you'll build and edit flowsheets, view graphs, and run and tweak process simulations.

When you first launch CHEMCAD, the workspace is solid white. When you start to build a flowsheet or open an existing simulation, the flowsheet displays in the workspace.

The workspace uses *tabs* to enable you to switch between your open simulation and any open Excel Data Maps and/or data plots. At the bottom of the workspace area, you'll see one or more tabs whenever a simulation is open. Each tab includes a button marked with an **x**; to close any tab, first click the tab and then click the **x** button.

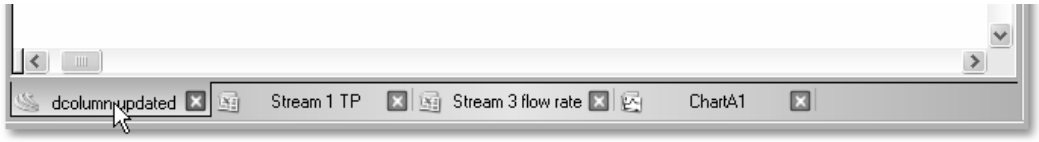


Figure 3-01: The bottom of the workspace area, showing several tabs and their x buttons

Note that any time you've closed a simulation and haven't yet opened another one, the workspace displays as a blank gray space.

The CHEMCAD Explorer Pane

Along the left edge of the CHEMCAD window, you'll see an area with a title bar at the top that reads *CHEMCAD Explorer*. At the bottom of the CHEMCAD Explorer pane are three tabs called **Recent Files**, **Simulation**, and **Visual Basic**. To view the contents of a tab, simply click its name.

Figure 3-02: CHEMCAD Explorer tabs

The CHEMCAD Explorer tabs are presented in what's known as a *tree format*, with items organized into a multi-level hierarchy. The default view shows only top-level items, but you can expand each item to view second-level items, third-level items, and so forth.

At the left of each top-level item is a small box with a plus sign. To expand an item, click the plus sign. Two things happen simultaneously when you click: the tree expands to show that item's contents, and the plus sign becomes a minus sign. You can hide (or *collapse*) the lower-level items again by clicking the minus sign, which then turns back into a plus sign. Figure 3-03 shows an example of a CHEMCAD Explorer item in collapsed and expanded view.

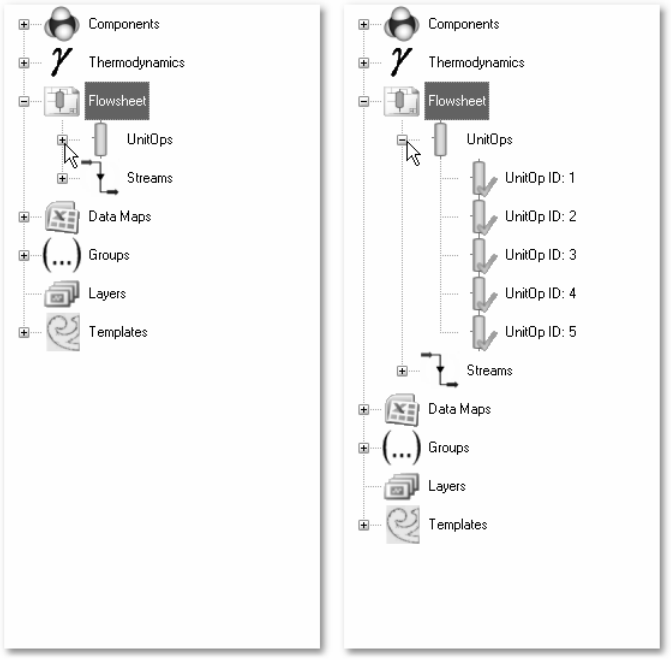


Figure 3-03: Clicking the plus sign to expand an item (left); the resulting view (right)

Expanding and collapsing items in the CHEMCAD Explorer tabs is one way that you can make the best use of your screen space when working in CHEMCAD.

The Recent Files Tab

The Recent Files tab is selected by default when you first launch CHEMCAD. This tab lists all of the simulation files that you have opened lately, starting with the most recent. When you first install CHEMCAD, the list is empty, but with every simulation that you open—new files or existing ones such as built-in examples—the list will grow, providing convenient access to files that you use frequently.

To open a simulation from the Recent Files list, simply double-click on the file name in the list.

The Simulation Tab

The Simulation tab displays by default any time a simulation is open. It provides a series of shortcuts to common commands and settings, including:

- **Components:** Includes one-click access to component, electrolyte, and solids selection, as well as distillation curves
- **Thermodynamics:** Provides quick access to thermodynamic settings and transport properties
- **Flowsheet:** Allows quick editing of UnitOp and stream data
- **Data Maps:** Enables you to create or set execution rules for a Data Map without using the menu

- **Groups:** Provides an easy way to categorize UnitOps, streams, and components
- **Layers:** Allows selected parts of the flowsheet to be displayed or hidden for viewing and printing
- **Templates:** Stores and organizes stream and UnitOp specifications that you can "clone" for re-use

Expand any of these items to see and use specific features, which are described in further detail in the appropriate chapters of this user guide.

The Visual Basic Tab

If you use Visual Basic to customize CHEMCAD, this tab provides quick and easy access to your Visual Basic code. You can expand the **Reactions**, **Properties**, or **UnitOps** item to view available subroutines for that category. Clicking the name of a subroutine opens a Visual Basic editor in a separate window.

The Palette Pane

Along the right side of the CHEMCAD window is a pane titled *Palette*, which is a repository for the various unit operation icons and other tools needed to draw flowsheets.

Selecting a Palette

These UnitOp icons and tools are grouped into *palettes* according to function or equipment type. The default palette is called **All UnitOps**, and it includes every available UnitOp icon and drawing tool. To select a different palette, simply click its title bar. The selected palette expands in place, as shown in Figure 3-04.

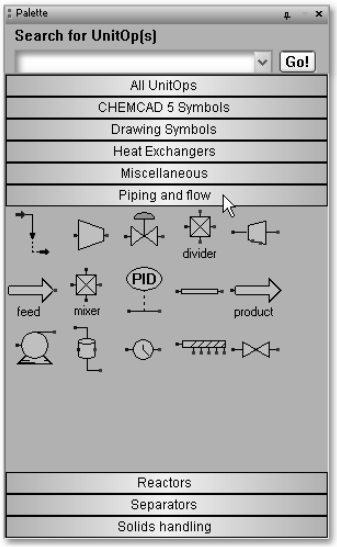


Figure 3-04: The expanded Piping and Flow palette

Customizing Palettes

At the top of the Palette pane is a field called **Search for UnitOp(s)**. Type a search term here and then click **Go!** to locate all of the UnitOp icons associated with that term. The results from the search appear in a new palette at the bottom of the Palette pane. Figure 3-05 shows the search results for the word **vessel**.

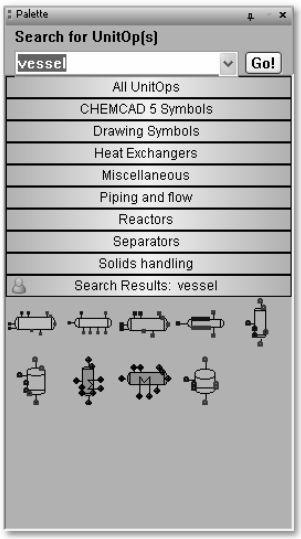


Figure 3-05: Search results showing all vessel UnitOps

Performing a UnitOp search creates what is known as a *user-added palette*. This type of palette is designated with a special icon at the left end of the palette heading.

The palette containing your search results remains available until you close CHEMCAD. You can make your user-added palette available permanently by right-clicking the new palette's title bar and selecting **Save**.

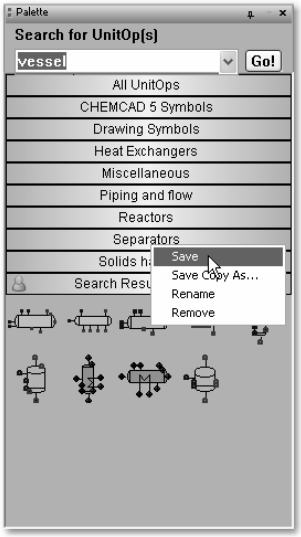


Figure 3-06: Saving search results for future use

You can do the following with user-added palettes:

- Rename any user-added palette by right-clicking its title bar and selecting **Rename**. In the resulting dialog box, type the name you want and then click **OK**.
- Delete a user-added palette at any time by right-clicking and selecting **Remove**.
- Add individual UnitOps or tools to an existing user-added palette. Simply right-click the icon for the item you want to add, select **Insert into Palette**, and then click the name of the user-added palette.
- Remove an item from a user-added palette by right-clicking the icon and selecting **Remove from Palette**.
- Create a user-added palette without a search. Right-click the first icon that you'd like to include on a new palette and select **Insert into Palette** > **New Palette**. Type a name in the resulting dialog box and click **OK**. Then add as many other icons as you'd like using the method described just above.

You cannot change the name or icon selection for a built-in palette, as you can with a user-added palette. You can, however, make a copy of a built-in palette, rename the copy, and then add and delete icons until the palette has just what you want.

To copy any palette (whether built-in or user-added), simply right-click the palette heading and select **Save Copy As**. Type a name for the new palette and click **OK**.

The Messages Pane

The Messages pane is located at the bottom edge of the CHEMCAD workspace. At the bottom of this pane are three tabs: **Errors and Warnings**, **Run Trace**, and **Notes**.

The Errors and Warnings Tab

This tab displays a running list of error and warning messages that have been generated while the current simulation file has been open. The oldest messages display at the top of the list. When there are too many cumulative messages to display in the pane, the most recent messages display and the older messages scroll off the top edge of the pane. If needed, you can use the vertical scroll bar on the right side of the pane to scroll up and review earlier messages.

The Run Trace Tab

This tab displays diagnostic messages from each UnitOp each time a simulation is run. This information is helpful in troubleshooting a simulation that is not working properly.

The text on the Run Trace tab is not saved with the simulation, but refreshes with each run and clears when you close the simulation.

The Notes Tab

This tab provides a handy place to store additional information, in text form, about the simulation. You can use it to list any details about the simulation, such as its origin and any assumptions that are being made.

Any notes that you add or change are saved as part of the simulation. To delete text from a note, simply click and drag to select the text and then press **[DELETE]** on your keyboard.

The Main Menu

The main CHEMCAD menu is located just under the title bar at the top of the program window. Some items on the main menu are common to nearly all Windows programs—namely **File**, **Edit**, **Format**, and **Help**—while other menu items such as **Thermophysical** and **Sizing** are more specific to chemical process simulation.

To use a menu command, click the relevant main menu item and then click the command in the drop-down list that appears.

To execute menu commands without using the mouse, you can hold down the **[ALT]** key on your keyboard as you press the letter key that corresponds to the underlined letter in the desired menu item, for example **[ALT-F]** for the File menu. You can then use the up and down arrow keys to select an item on the menu and press **[ENTER]** to execute the selected command.

The Toolbar

The CHEMCAD toolbar provides buttons that are common to most Windows applications, such as **New**, **Open**, **Save**, and **Print**, along with buttons that are specific to chemical process simulation.

To discover the use of a particular button, simply point your mouse cursor at the button and watch for the tooltip to appear, as shown in Figure 3-07.

Figure 3-07: Viewing a button's tooltip

Toolbar buttons provide quick, one-click access to frequently-used commands that are also available via the CHEMCAD menus.

Customizing the CHEMCAD Screen

When you first install CHEMCAD, the screen is laid out with the CHEMCAD Explorer pane on the left, the Palette pane on the right, and the Messages pane below the workspace.

If having all of these items visible leaves you less workspace than you would prefer, or if the location of one or more panes is less than optimal for the way that you work, you can hide or move panes to customize your CHEMCAD screen.

Viewing and Hiding Screen Elements

You can view or hide any of the CHEMCAD screen's panes, as well as groups of toolbar buttons, to make optimal use of your screen space.

To toggle a pane on or off, select the **View** menu and then choose **CHEMCAD Explorer**, **Palette**, or **Messages**. Items with a check mark are currently displayed, while items with no check mark are currently hidden. You can also choose to view or hide the status bar at the bottom of the CHEMCAD window.

To selectively view or hide groups of toolbar buttons, select **View** > **Toolbars**. In the Toolbars dialog box, each group of buttons is listed under a descriptive name; initially, all of these groups have check marks, indicating that they are currently displayed. To hide any group of buttons, click to remove the check mark and then click **Close** to return to the main CHEMCAD window.

Resizing and Moving Items

Now that you have determined which panes and toolbar button groups to display, you can further customize your CHEMCAD window to determine exactly where each of these items will appear.

Resizing a Pane

The simplest way to alter the appearance of a pane is to resize it. You can make the CHEMCAD Explorer and Palette panes wider or narrower, or make the Messages pane shorter or taller, by moving the inside edge, or *wall*, of the pane toward or away from the edge of the main window.

To resize a pane, start by positioning your mouse cursor at the inside wall of the pane—that is, the right edge of the CHEMCAD Explorer pane, the left edge of the Palette pane, or the top edge of the Messages pane. When the cursor is in the correct position for resizing, the normal pointer will be replaced with a two-headed arrow as shown in Figure 3-08.

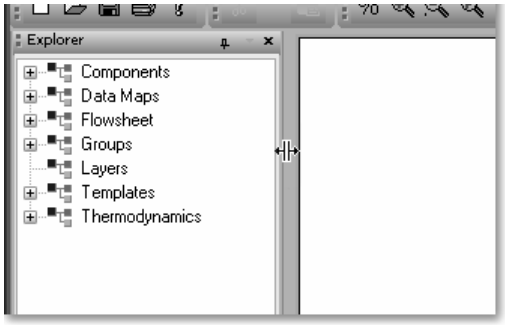


Figure 3-08: The two-headed arrow cursor used for resizing panes

When you see the two-headed arrow, click and drag in the direction you want to move the pane wall. A thick gray line shows a preview of the new pane size; when you release the mouse button, the resized pane appears.

Moving a Pane

In addition to resizing, you can also move any of the panes in the CHEMCAD window, either to a different edge of the screen or to the middle of the screen. You can also move groups of buttons from their default positions on the toolbar.

Initially, all of the panes and button groups are *docked*, meaning that they are "snapped into" an edge of the screen or the toolbar area. When you *undock* an item, you can put it in the location of your choosing, away from the screen edge.

To undock a pane, click and drag the pane's *title bar*, that is, the blue bar at the top of the pane that shows the pane name. To undock a button group, you'll need to click and drag the row of four dots running along the left edge of the leftmost button in the group.

Note: In the case of the Messages pane, the title bar runs along the left edge of the pane, and the name is not visible when the pane is docked.

If you drag the pane or button group into the workspace area, you'll see a gray box representing the position the item will occupy when you release the mouse button. If you don't like the new position, you can click the item's title bar and drag it elsewhere, including its original position.

You can also dock a pane to a different edge of the screen, or move button groups around within the toolbar area, instead of undocking these items.

Pinning and Unpinning Panes

In addition to moving and resizing the various panes, there's another way that you can customize your CHEMCAD screen: *pinning* and *unpinning* the CHEMCAD Explorer and Palette panes.

These two panes can take up a fair amount of horizontal screen space, and making them very narrow isn't an ideal way to work. Pinning and unpinning provide a way to view full-width CHEMCAD Explorer and Palette panes when you need these tools, while also freeing up space when you aren't using them.

Whenever either of these panes is docked at an edge of the screen, it is in one of two states:

- Pinned, meaning that the pane is always visible
- Unpinned, meaning that the pane is mostly hidden from view, and appears only on demand

By default, all CHEMCAD panes are initially pinned in place. You can choose to unpin a pane if you prefer to have some extra space on the screen. To unpin a pane,

find the tiny pushpin icon in the pane's title bar, next to the **x** icon that enables you to close the pane. If the pane is stationary, you'll see that the pin is upright with its point down.

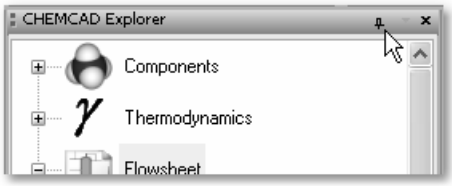


Figure 3-09: The icon indicating a pinned, or stationary, pane

If you click the pin icon, the pane suddenly disappears from view—but it isn't gone. Instead, a small gray tab bearing the name of the palette appears at the edge of the screen where the pane is docked. To see the pane reappear, you only have to roll your mouse over that tab. When the pane appears, you'll notice that the pushpin icon is now pointed to the side. Use the tools on the CHEMCAD Explorer or Palette normally; then, when you no longer need the pane, just move the mouse pointer elsewhere. The pane will automatically hide itself until the next time you roll the mouse over the tab.

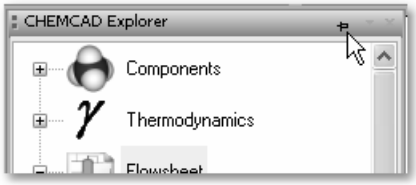


Figure 3-10: An unpinned pane in use; note the sideways pin icon

To re-pin an unpinned pane, point to the tab to make the pane appear and then click the pin icon. The pin turns so that it is once again upright, and the pane is once again a permanent fixture on the CHEMCAD screen.

Other Useful Interface Hints

The following are helpful items that can help to make your CHEMCAD experience easier and more efficient.

Undo and Redo

As with most Windows-based programs, CHEMCAD allows you to "back out" of actions you have just taken while working with a file. You can use the Undo command to negate the last change you made; simply select **Edit** > **Undo,** or use the key combination **[CTRL-Z]**.

You can use the Undo command to retract up to the last 99 actions that you performed since the last time you opened the current simulation file.

Visible Grid

You can turn on a workspace grid to use as a guide while creating your flowsheet. Select **View** > **Grid Visible** to toggle this feature on or off.

Other grid options include **View** > **Snap to Grid**, which helps with alignment of objects on the flowsheet, and **View** > **Change Grid Size**, which enables you to customize the horizontal and vertical spacing of grid lines.

Adjusting Your View of the Workspace

The **View** > **Zoom Options** menu offers a whole series of options for moving and resizing your view of the CHEMCAD workspace.

- Select **In** to view the workspace from closer in, or **Out** to view from farther away.
- Select either **In at a Point** or **Out at a Point**, and then click a point on the workspace, to zoom in or out with that point as a focus.
- Select **Zoom Rectangle**, and then click and drag on the workspace, to designate a specific area that you want to view.
- Select **Zoom Percentage** to choose a specific display size for the workspace.
- Select **Zoom to Fit** to view at the largest size that still permits all of the existing flowsheet elements to remain in the visible workspace.

If your computer mouse is equipped with a scroll wheel between the left and right mouse buttons, you can zoom in and out on the CHEMCAD workspace with a touch of your finger. To zoom in, roll the wheel up—that is, push your fingertip away, toward the top edge of the mouse. To zoom out, roll the wheel down toward the bottom of your mouse, pulling your fingertip toward your palm.

Note: When you zoom in and out using the scroll wheel, the focal point for the zoom is the location of the mouse pointer.

The CHEMCAD Coach Pane

The CHEMCAD Coach pane is not displayed by default, but you can access it at any time by selecting **Help** > **CHEMCAD Coach**. The purpose of CHEMCAD Coach is to provide concise instructions for common procedures. If you've learned how to perform a common procedure in CHEMCAD but have forgotten the exact menu command to use, CHEMCAD Coach can help jog your memory and put you on the right track.

You can drag the CHEMCAD Coach window to any location on the screen, simply by clicking and dragging the title bar at the top of the window.

If you have finished using the CHEMCAD Coach tool and want to close it, just click the **Close** button (the red **X**) in the upper right corner of the CHEMCAD Coach window. Note that if the main CHEMCAD window was maximized before you opened the CHEMCAD Coach tool, you may need to maximize the CHEMCAD window again to restore it to full-screen size.

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Chapter 4

Working with Simulation Files

All of the work that you do with CHEMCAD is stored in simulation files. With the advent of CHEMCAD 6, each discrete simulation is packaged into a single file that is portable and easy to handle. All the details of the simulation—from UnitOp specifications to stream composition to thermodynamics—are included in this file. This chapter describes the various ways that you can access and manage CHEMCAD simulation files.

About CHEMCAD Simulation Files

Simulations created in CHEMCAD 6 use the file extension .CC6, which distinguishes them from other files on your computer, including simulation files created using earlier versions of CHEMCAD.

One of the most notable differences between .CC6 files and predecessors such as .CCX files is their portability. A .CC6 simulation file is as easy to work with, transport, and share as an MS Word document or an Excel spreadsheet. Whereas CHEMCAD simulations once required extra steps before they could be e-mailed or moved, simulations created with CHEMCAD 6 can be handled as stand-alone files.

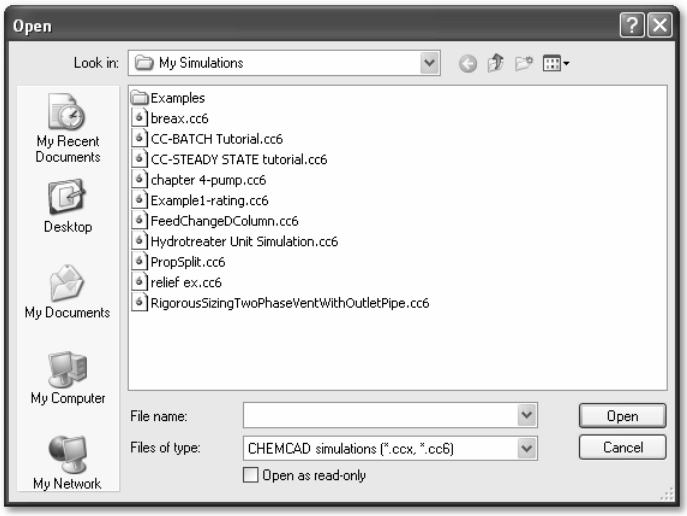


Figure 4-01: Stand-alone CHEMCAD 6 files in the My Simulations directory

User Components in CHEMCAD

Another departure from previous versions of CHEMCAD is that simulations are now self-contained with respect to the data needed to run them. All custom components that you create are stored in a database so that you can use them in many different simulations. User components are also stored within the simulations that use them, so you no longer have to worry about losing user components when moving a simulation from place to place.

Each time you open a simulation, CHEMCAD compares any user components in the simulation with the copies of those same components in the database. If the two copies do not match, you will be offered a choice: you can keep using the local copy stored in the simulation, or use the updated copy from the database.

Your copy of CHEMCAD can now have multiple user databases, and even share them on networks with other users. To learn more about user components and best practices for managing and securing user component databases, see Chapter 10, *Customizing CHEMCAD*.

Example Files

Especially if you're new to CHEMCAD, it's a good idea to open and practice working with some example files before creating your own simulations. For this purpose, we've created numerous examples of simulations for typical chemical processes. You can open, view, and edit any example file, and even save a copy in another location to jump-start a simulation of your own.

The CHEMCAD example files are automatically copied to your computer with a complete CHEMCAD installation. The examples are organized by process type and located in the **\My Documents\My Simulations\Examples** directory.

Opening an Existing Simulation

Select **File** > **Open** to bring up the Open dialog box. Navigate to the folder where the simulation is located, select the appropriate .CC6 file, and click **Open**.

If you use CHEMCAD on a network and share files with other users, it's possible that you could try to open a simulation that is already open for editing by another user. If you should attempt to open a simulation that is unavailable for editing, a message box will appear. You can choose to save the simulation with a new name and/or location, open a read-only copy of the simulation, or cancel the open operation.

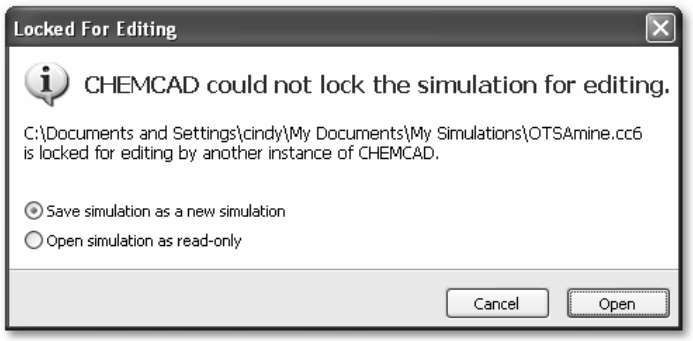

Locked For Editing
CHEMCAD could not lock the simulation for editing.
C:\Documents and Settings\cindy\My Documents\My Simulations\OTSAmine.cc6
is locked for editing by another instance of CHEMCAD.
Save simulation as a new simulation
Open simulation as read-only
Cancel
Open

Figure 4-02: Notification that a simulation is already in use

If you should have trouble locating a particular simulation, you can search your hard drive or network for all files with a .CC6 file extension.

Creating a New Simulation

When you first open CHEMCAD, you'll see a blank simulation window and **[Untitled]** in the title bar.

You can begin building your simulation right away, but it's recommended that you save and name the simulation before you proceed very far. The longer you wait to save the simulation, the more you risk losing your work if an unforeseen computer or network problem should occur.

If you already have a simulation file open and want to start a new simulation, first save your work if applicable. Then select **File** > **New** or click the **New** toolbar button, to close the current file and bring up a new blank simulation screen. Note that if you have unsaved changes in your existing file, CHEMCAD will ask you to save or discard your changes before opening the new simulation.

Saving a Simulation

To save all changes in a simulation that you have already named, select **File** > **Save** or click the **Save** button on the toolbar.

Note: In some cases, such as the built-in CHEMCAD example files, existing files may be set as read-only to prevent accidental overwriting. You can save a copy of a read-only file using a different file name and/or file location.

To save a new simulation that you haven't yet named, select **File** > **Save As**. The Save As dialog box appears, with **CHEMCAD 6 (*.cc6)** as the default file type. Leave the file type as it is, give the file a unique name, and if necessary navigate to a new file location. Click **Save** to close the dialog box and return to the saved simulation.

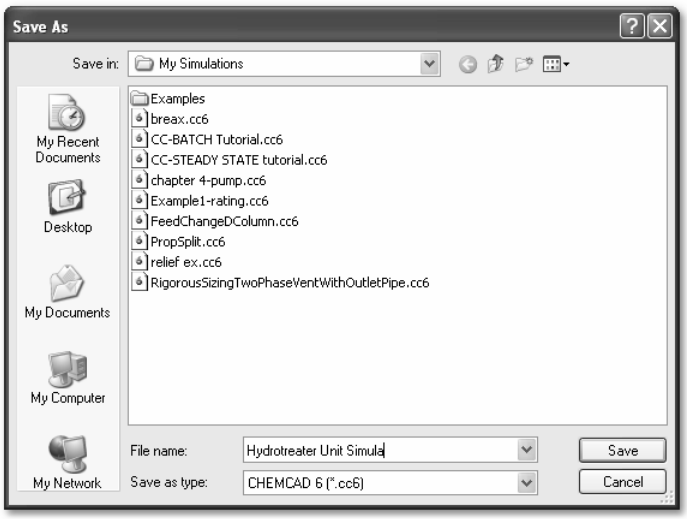


Figure 4-03: Giving a new simulation a unique name

Note: Unlike previous versions of CHEMCAD, the changes you make to a simulation are not saved until you use the **Save** or **Save As** command. This offers you greater flexibility in choosing which changes to save or discard.

Saving and storing all of your simulations in the same directory helps prevent the lost time and frustration that can result when files are scattered in different locations. It is recommended that you store your simulations in the **My Simulations** folder, which is created automatically within the **My Documents** folder at installation.

Saving Different Cases for the Same Simulation

In certain situations, you may need to create a group of simulations that are nearly identical to one another; previous versions of CHEMCAD referred to such groups of similar simulations as *cases*. In CHEMCAD 6, each simulation is a free-standing file, but you can still easily "clone" simulations and make minor changes for comparison cases.

To do this, simply create a simulation, save it, and then select **File** > **Save As** to rename the next case. Make the needed changes for that case, save it, and continue in that vein to create as many clones of your original simulation as needed, with whatever differences you require.

E-mailing a Simulation

With CHEMCAD 6, e-mailing a simulation is a simple matter of adding a file attachment. Just open your preferred e -mail program, create a new message, choose your recipients and add your text, then use the program's command for attaching a file. Navigate to the folder where the simulation is located, select the appropriate .CC6 file, and add the file as an attachment.

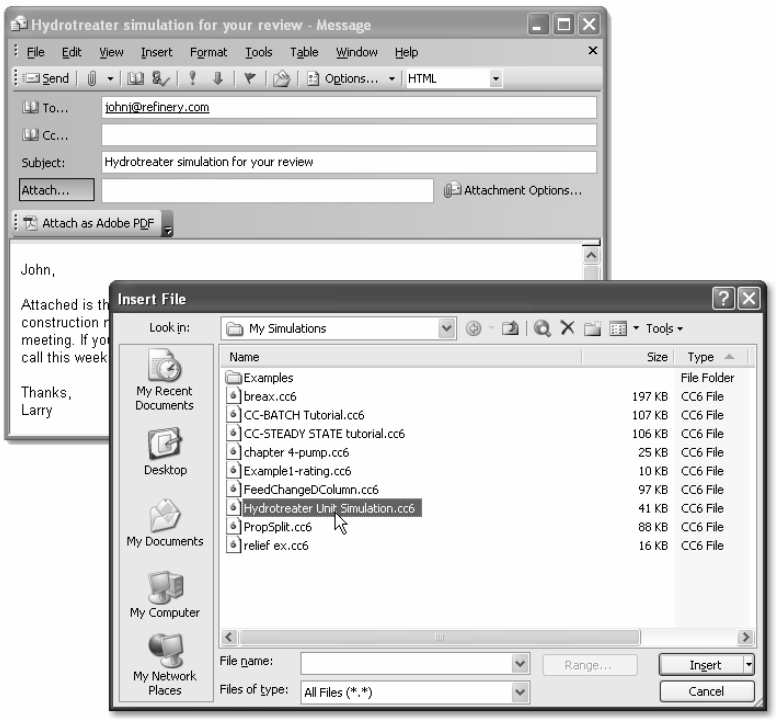


Figure 4-04: Adding a .CC6 file as an attachment in MS Outlook

Before you e-mail a simulation, you should ensure that you have saved any recent changes. Also, it's a good idea to check the size of the file before adding the attachment, as simulation files can in some cases be quite large.

Working with CHEMCAD Files from Previous Versions

You can use CHEMCAD 6 to open simulations that were originally created with CHEMCAD 5. When you do this, CHEMCAD creates a copy of the original simulation, and makes that copy compatible with all CHEMCAD 6 functionality. The flowsheet and simulation data in the copy are not altered in any way, and the original file is left intact.

To bring an existing simulation up to date with CHEMCAD 6, select **File** > **Open**, select the simulation, and click **Open**. A message will appear, notifying you that the simulation will be copied.

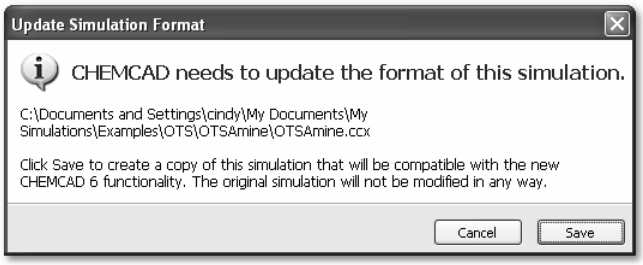

Update Simulation Format
CHEMCAD needs to update the format of this simulation.
C:\Documents and Settings\cindy\My Documents\My Simulations\Examples\OTS\OTSAmine\OTSAmine.ccx
Click Save to create a copy of this simulation that will be compatible with the new CHEMCAD 6 functionality. The original simulation will not be modified in any way.
Cancel
Save

Figure 4-05: Converting a CHEMCAD 5 file to the .CC6 format

Click **Save** to bring up the Save As dialog box, where you can either keep or change the file's name and select a location for the CHEMCAD 6 copy. Click **Save** to create and open the new file.

Chapter 5

Building and Using a Basic Simulation

Although the types of simulations you can create using CHEMCAD are many and varied, the basic procedure for creating a simulation can be broken down into the following common steps:

1. Start a new simulation.
2. Select engineering units for the simulation.
3. Create a flowsheet with the appropriate streams and unit operations.
4. Select chemical components for the process.
5. Select K-value and enthalpy options for the process.
6. Define the feed streams used in the process.
7. Enter specifications for the unit operations.
8. Run the simulation.
9. Review the results of the simulation.

Starting a New Simulation

Launch CHEMCAD and then select **File** > **Save As**. In the Save As dialog box, specify a name and location for the simulation file.

When you first install CHEMCAD, the default location for saving new simulations is a folder called **My Simulations**, located within your computer's My Documents folder. You can save your new simulation to that folder, or to any accessible directory on your computer or network. As you'll notice in the Save As dialog box, the file extension for CHEMCAD simulation files is **.CC6**.

Selecting Engineering Units

To specify engineering units for this simulation, select **Format** > **Engineering Units**. This brings up the Engineering Unit Selection dialog box, where you can select the units to be used for everything from time and temperature to surface tension. The majority of the options in this dialog box are located on the **Units selection** tab, but you can click a second tab called **Options and references** for more options.

The buttons along the bottom of the **Units selection** tab enable you to set all of the units to English, alternative SI, SI, or metric. If your desired units do not fit neatly into one of these categories, you can choose the closest one and then manually select different units for any items you like.

If you do find yourself customizing your list of units, you can save your selections as a set, or *profile*, that you can quickly duplicate for future simulations. To do this, first set all of the units the way you want them, then type a name for this profile and click the **Save Profile** button.

You may not notice anything happening when you click **Save Profile**, but you can verify that your new profile has been saved by clicking the **Load Profile** button. This is the button that you will use for future simulations, to apply your custom units profile with a single click. You should see a Select Item screen that shows the name you gave the profile. If you click the profile name and then click **OK**, you'll load your custom units profile.

Back on the Engineering Unit Selection dialog box, click **OK** to apply your engineering unit selections and continue creating your simulation.

Drawing the Flowsheet

To create the flowsheet for your simulation, you'll need to add the appropriate unit operation icons to your workspace and connect those UnitOps to one another with streams. This connected group of streams and UnitOps forms the basis for the simulation.

The tools for drawing a flowsheet are located in the Palette pane, which by default displays on the right margin of the CHEMCAD window. The Palette pane is divided into UnitOp categories, or you can view all of the available UnitOp icons at once using the All UnitOps view.

Adding UnitOps

To place a UnitOp icon on your flowsheet, follow these steps:

1. On the All UnitOps palette, find the appropriate UnitOp icon for the equipment you want to represent. When you point to the icon with the mouse, the box around the icon lights up. Click the icon to select the UnitOp.
2. Move your mouse cursor to the workspace area, noting that the pointer displays an outline of the UnitOp icon you've selected. Point to the location

on the workspace where you want to place the selected UnitOp, and then click and release the left mouse button. The icon for the selected UnitOp appears where you clicked.

3. Right-click to deselect the UnitOp drawing tool and return to a normal pointer. You can now click in the workspace area without drawing duplicate UnitOps.

Selecting a Default Icon for a UnitOp

For certain UnitOps, you can select a default icon to customize the way that type of equipment looks on your flowsheet.

> **Note:** Icons that are already in place on the flowsheet will not be affected when you select a new default icon.

You can see which icons offer this feature by moving your cursor over the All UnitOps palette, noting the boxes that light up around the icons. A UnitOp that offers a choice of default icons will have a black triangle in the lower right corner when you point to its box.

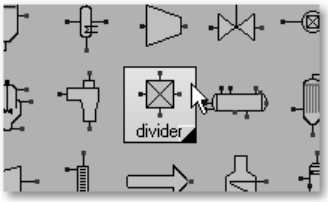


Figure 5-01: Black triangle showing that the Divider UnitOp offers a choice of icons

To select a new default icon for a UnitOp, click the black triangle to see a pop-up selection box with all available icons. Click the icon you want to use; that icon replaces the previously displayed icon on the palette. You can change the default icon for a UnitOp as often as you like.

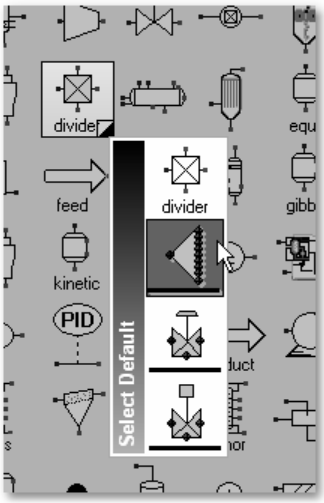


Figure 5-02: Selecting a new default Divider UnitOp icon

Manipulating UnitOp Icons

After drawing a UnitOp icon on a flowsheet, you can move, resize, or delete the icon as needed.

1. Verify that the mouse pointer currently displayed is a normal arrow. If the pointer displays as a UnitOp icon outline, right-click to turn off UnitOp drawing.
2. Click the UnitOp icon so that its four sizing handles (black boxes at each corner) appear.
3. Manipulate the UnitOp icon as needed:
   - To move the UnitOp, click the icon and drag to its new location.
   - To resize the UnitOp, click any sizing handle and drag inward or outward to achieve the desired size.
   - To delete the UnitOp, right-click and select **Delete**, or simply press the **[DELETE]** key on your keyboard.

Drawing and Connecting a Stream

Before you can add a stream to a flowsheet, you must already have drawn the UnitOps that the stream will connect. Follow these steps to add a stream:

1. Click the **Stream** tool in the upper right corner of the All UnitOps palette.
2. Move the cursor onto the workspace, noting that the pointer now appears as a small plus sign. Find the icon for the UnitOp where the stream will start, and point at the icon so that the blue inlet dots and red outlet dots are visible. If this UnitOp offers more than one outlet location, decide which one you will use.
3. Point at the red outlet dot so that the pointer turns into a small black arrow. Click and release the left mouse button to start drawing the stream.
4. Move the cursor toward the UnitOp where the stream will end. As you approach the UnitOp icon, the inlet and outlet dots on that icon will become visible. If more than one inlet location is available, decide which one you will use.
5. When you reach the blue inlet dot, click the mouse again to complete the stream.

After you draw a stream, the Stream tool remains active so that you can draw another stream right away if desired. To turn off stream drawing, simply click on any blank area of the workspace; this returns your pointer to the normal white arrow, which you can use to select and manipulate items on the flowsheet.

Choosing a Stream Route

If you draw a stream by clicking only at the UnitOp outlet and inlet, CHEMCAD chooses the shortest and most direct path for the stream. In some situations—when a UnitOp is in the direct path of the stream, for example—you will need to choose a deliberate route for your stream.

To do this, click the mouse as you move from outlet to inlet, wherever you want the stream to make a turn. Each time you click, the stream freezes in place, and from there you can make a 90° turn to either the left or the right. You can add as many detours as you like to a stream before bringing it into a UnitOp inlet.

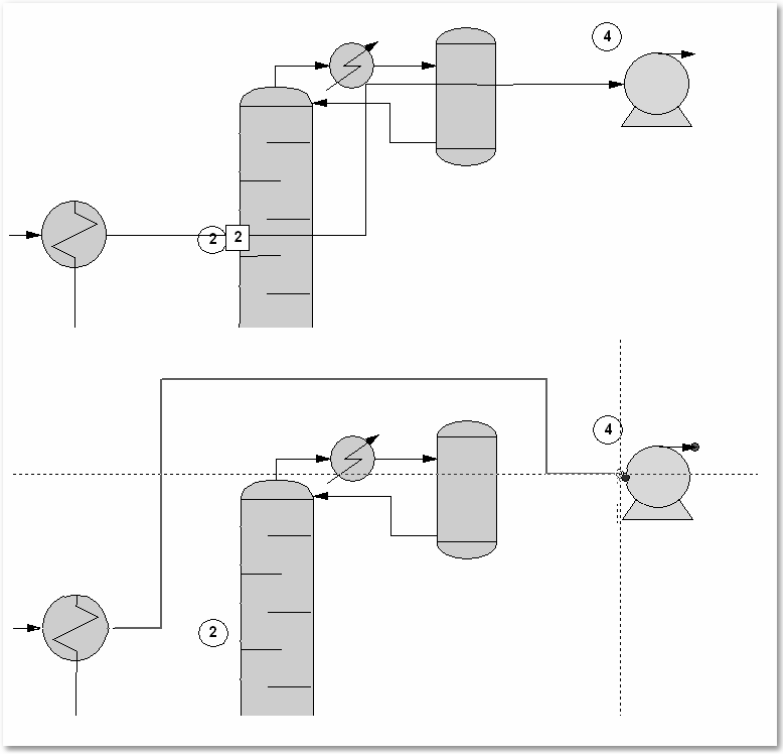


Figure 5-03: Stream 2 with automatic routing (above) and deliberate routing (below)

Rerouting a Stream

Even after you've completed your flowsheet and added detailed information about your streams, you can still reroute a stream if needed. To do this, click the stream to select it, then right-click and select **Reroute stream**. The old stream disappears, replaced by the beginning of a new stream originating at the same outlet.

You can now click to create 90° turns, the same way you would with a new stream, to route the stream exactly where you want it. Your last click must complete the stream at the same inlet you used before. After a stream is rerouted, it retains all of the stream detail that you had previously entered.

Other Drawing Tools

In addition to the Stream tool and the various UnitOp icons, the Palette pane offers a text tool, as well as tools for drawing rectangles, ellipses, lines, multi-part lines, and polygons.

The Text Tool

To place text on a flowsheet, select the Text tool (which displays a large letter T) on the All UnitOps palette. When you move your cursor over the workspace, you'll now see that your pointer has become a vertical line. Click the mouse to place a blinking cursor on the flowsheet.

Start typing the text that you want to add. You will see the text appear wherever you clicked the mouse. When you finish, click anywhere in the workspace to turn off the Text tool.

You can now click and drag your new block of text around the workspace. You can also select **Format** > **Color** or **Format** > **Font** to access various standard text and object formatting tools.

Simple Drawing Tools: Rectangle, Ellipse, and Line

You can draw various shapes as needed on a flowsheet. The simplest of these shapes to draw are rectangles, ellipses, and lines.

To add any of these shapes to a flowsheet, simply click the corresponding tool in the All UnitOps palette. Then, then click and drag in the workspace to draw the shape, releasing the mouse button when you have achieved the desired size and shape.

Note that to make a perfect square or circle, you can hold down the **[SHIFT]** key as you draw with the Rectangle or Ellipse tool, respectively.

Complex Drawing Tools: Multi-line and Polygon

In addition to these straightforward, click-and-drag shapes, you can also create more complex shapes and lines on a flowsheet.

To create any open figure with an irregular shape, select the **Multi-line** tool in the All UnitOps palette. Move your cursor to the workspace and click in the area where you want to start drawing. Then move the cursor and click again to create the shape's first line. Keep clicking and moving the mouse until you've created the shape you want, and then double-click to complete the shape and turn off the Multi-line tool.

To create an irregular closed polygon, select the Polygon tool and then move your cursor to the workspace. Click where you want to start drawing, and then click a second time to create the first side of your polygon. After the second click, you'll begin to see the open area being created. Continue moving the cursor and clicking until you are ready to place your last point, and then double-click to complete the shape and turn off the Polygon tool.

Note that you can hold down the **[SHIFT]** key while using the Polygon tool to create a right triangle.

Selecting Chemical Components

You can select chemical components for your simulation at any point while creating the flowsheet, or you can wait until you've drawn the entire flowsheet before adding components. Before you can run the simulation, you will need to list every component involved in your chemical process so that CHEMCAD can work with those components' properties.

These chemical components are pulled from CHEMCAD's *component database*, a master list of thousands of chemicals with their associated properties. When you're ready to list components for your simulation, select **Thermophysical** > **Select Components** to open the Select Components dialog box.

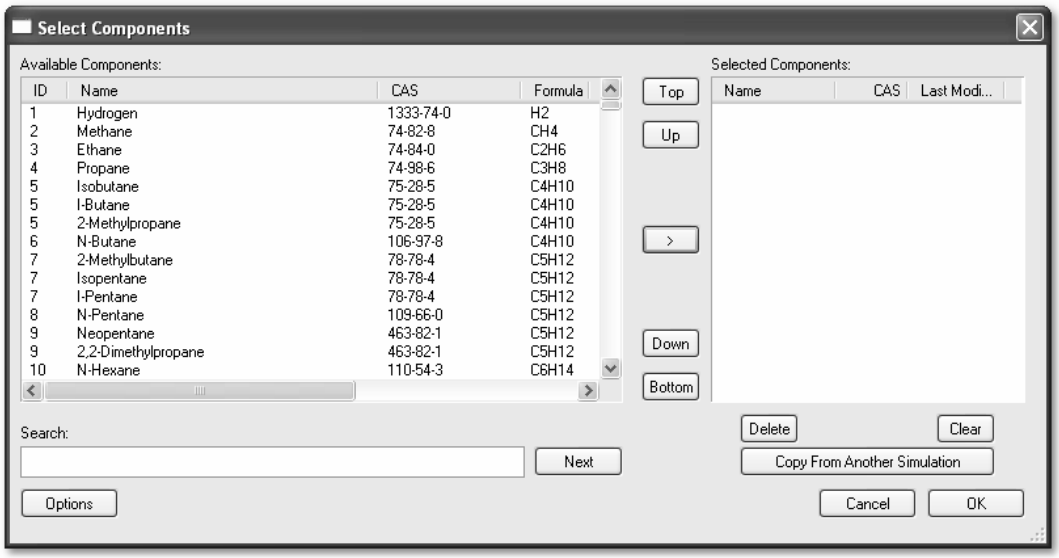


Figure 5-04: The Select Components dialog box

The Available Components column lists the contents of the CHEMCAD component database, while the Selected Components column lists the components currently included in this simulation. For a new simulation, the Selected Components list is empty at first.

Every chemical that will be part of the process, whether it's a feed stream, product, or utility, must be listed on this simulation's component list.

Finding a Component

Because of the large number of components in the CHEMCAD component database, scrolling up and down the list of available components can be time-consuming. To find a specific component quickly, use the Search box at the bottom of the Select Components dialog box.

Type the name of the chemical you want to find in the Search box. With each letter that you type, CHEMCAD suggests possible matches in the Available

Components list. In the following example, typing the letters **wa** in the Search field has highlighted the **Water** component.

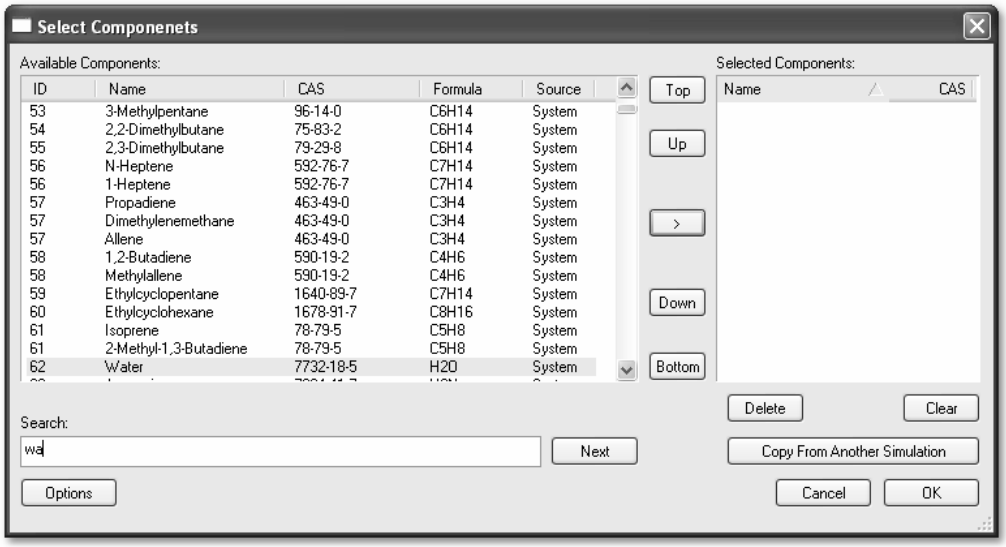


Figure 5-05: Using the Search box to locate the Water component

The Search field accepts both text and numeric entries. By default, CHEMCAD will search for your entry among all chemical names, chemical formulas, CHEMCAD database IDs, and CAS numbers. If you would prefer not to search this broadly, click the **Options** button. This brings up a dialog box that enables you to "opt out" of including any of these items in your searches.

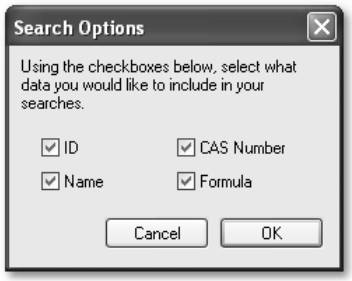


Figure 5-06: Selecting what to include in component searches

Note: You can add your own custom components to the CHEMCAD component database. For more details about this feature, see Chapter 10 of this manual.

Adding a Component

Once you've located the component you want in the Available Components list, simply double-click the component to add it to the Selected Components list for your simulation.

You can also select multiple components in the Available Components list and then click the right arrow button, located between the two columns, to add the components to your simulation. To select multiple components, use Windows' standard selection methods of holding down **[SHIFT]** to select contiguous items or holding down **[CTRL]** to select non-contiguous items.

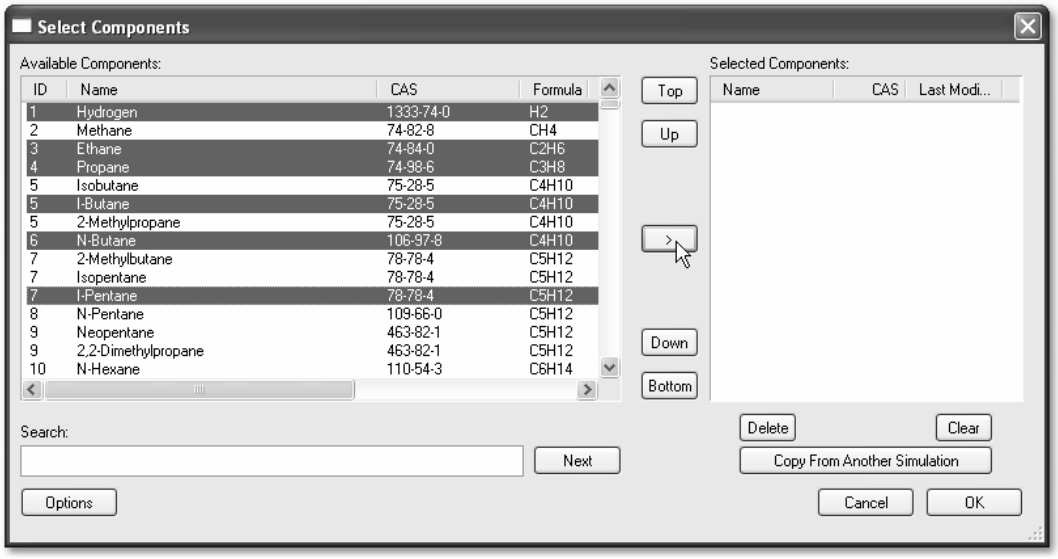


Figure 5-07: Adding multiple components using the right arrow button

If you would like to duplicate the component list from an existing simulation, click **Copy From Another Simulation**. In the resulting Open dialog box, navigate to the desired simulation, select that simulation, and click **Open**. The Selected Components list is now populated with the components used in the simulation you selected; you can add or delete items to customize the list.

Changing the Order of Selected Components

When your Selected Components list for a simulation is particularly long, you may find it helpful to place certain components at either the top or the bottom of the list. You can add components in any order, and then move them around in the list as needed.

To move a component to a new position in the Selected Components list, click the component to select it and then:

- Click **Top** to move it to the first position on the list.
- Click **Up** to move it up one position.
- Click **Down** to move it down one position.
- Click **Bottom** to move it to the last position on the list.

Removing Items from the Selected Components List

To remove a single component from the Selected Components list, click the component to select it and then click **Delete** in the bottom right area of the Select Components dialog box.

To remove all components from the Selected Components list and begin again, click **Clear**, just to the right of **Delete**. If you have changed your mind about adding components at this time, you can simply click **Cancel** to back out of component selection.

Selecting K-value and Enthalpy Options

The first time you complete the Component Selection dialog box, you'll be taken to the Thermodynamics Wizard dialog box. At this point, you can either click **Cancel** to skip the wizard and enter thermodynamics manually, or enter parameters in the dialog box and click **OK** to see which methods the wizard suggests.

Using the Thermodynamics Wizard

Proper selection of thermodynamics is generally the most important step in a process simulation. A poor thermodynamics selection may lead to unrealistic simulation results.

The Thermodynamics Wizard makes general suggestions, based on your component list and the specified ranges for temperature and pressure.

Selecting Components to Ignore

In the upper portion of the wizard screen, use the drop-down boxes to indicate any components that the Thermodynamics Wizard should *not* consider. This may affect the results for model suggestion. For example, if you are using water as a coolant and your other components are alkanes, the Thermodynamics Wizard will choose UNIFAC. If you specify that water should be ignored, the wizard will ignore the water and select SRK.

Specifying Process Conditions

In the lower portion of the wizard screen, specify the approximate temperature and pressure ranges for this process. Entering accurate information in these fields will help the Thermodynamics Wizard return a more useful recommendation.

In the BIP Data Threshold field, enter the minimum percentage of possible binary interaction parameters (BIPs) which must be present in a BIP activity coefficient model (NRTL, Wilson, etc). Without BIPs, activity coefficient models simplify to Raoult's law.

How the Thermodynamics Wizard Makes Suggestions

CHEMCAD's Thermodynamics Wizard follows a logic tree to choose a model. The logic tree assumes that all your components are mixed in a vessel, with conditions falling into the specified temperature and pressure ranges.

- If all components are hydrocarbons, the wizard will likely suggest an equation of state.
- If water is present, the wizard will likely select an activity coefficient method.
- If water and hydrocarbons are present, the wizard will likely select UNIFAC.
- If water and strong electrolytes (HCl, NaOH, etc.) are detected, the wizard will suggest electrolyte models.

Temperature and pressure range will affect the selection of model. If pressure is high, CHEMCAD is more likely to suggest an equation of state. If pressure is atmospheric and temperature is below the normal boiling point of all components, CHEMCAD may choose a liquid activity model or ideal vapor pressure.

Should the Thermodynamics Wizard be trusted to make design decisions?

Use the wizard as a starting point for your decision. Proper selection of thermodynamics is the engineer's responsibility. Your simulation may call for the use of a different thermodynamic model than what the Thermodynamics Wizard suggests.

Manually Selecting Thermodynamics Settings

To set up thermodynamics for your simulation manually, follow these steps:

1. Select **Thermophysical** > **Thermodynamic Settings**, or click the button by the same name on the toolbar.

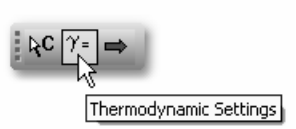


Figure 5-08: The Thermodynamic Settings button on the toolbar

2. This opens the Thermodynamic Settings dialog box. Start by determining, based on your process knowledge, whether your system has two liquid phases or a single liquid phase. In the **Global K Value Option** field, select a method that can calculate the phase behavior relevant to your system.
3. Based on the specific circumstances of your process, make any needed alterations to the options displayed on the **K-value Models** tab. Note that the options appropriate to your selected K-value method are displayed in black, while irrelevant options are displayed in gray.
4. Click **Enthalpy Models** tab, select the most appropriate model in the **Global Enthalpy Option** field, and make any other changes to the options on this tab as needed for your process.
5. Click the **Transport Properties** tab and verify that the settings there are appropriate for this simulation. Change any settings as needed and then click **OK** to close the Thermodynamic Settings dialog box.
6. If you've made any changes, a message box appears: *All streams should be reinitialized. Proceed with reinitialization?* Click **Yes** to reinitialize all streams now, or **No** if you'd prefer to wait and reinitialize the streams later.

Defining Streams

The streams that you have drawn on your flowsheet are still just lines with no data behind them, so the next step is to edit these streams, populating them with composition data and other properties.

> **Note:** In most situations, the streams you'll need to define will be the feed streams in your process. Other types of streams, such as recycle cut streams, may also require definition.

You can edit a single feed stream using either of these methods:

- Double-click the stream.
- On the **Simulation** tab in the CHEMCAD Explorer, expand **Flowsheet** and then **Streams**, right-click the stream in question, and select **Edit Stream**.

You can edit all feed streams in the flowsheet at once using either of these methods:

- Select **Specifications** > **Feed Streams**.
- Click the **Edit Feed Streams** toolbar button, which displays a large red feed stream arrow.

Whichever method you choose, you'll see the Edit Streams dialog box, with either a single column of data or a column for each feed stream in the flowsheet. In this dialog box, specify properties for each feed stream listed.

Thermodynamic Properties

You must specify exactly two of the following three variables:

- Temp F
- Pres psia
- Vapor Fraction

CHEMCAD will calculate the third variable and enthalpy, based on the two variables you specify and the thermodynamics method you've selected.

Stream Composition

To define the stream composition, you'll need to specify a composition unit and the amount of each component that is present in the stream.

Select a unit from the **Comp unit** drop-down list, and then based on that selection, populate the field for each component with the appropriate amount, percentage, or fraction.

For stream compositions expressed as a percentage or fraction, you can enter values that do not total 100%. In this case, CHEMCAD will normalize the

composition to fractional values that total 1. To preview the normalized values that CHEMCAD assigns to the components, click **Flash**.

Total Flow Properties

If the component flow engineering unit used for a stream is dimensionless (i.e., mole fraction, weight fraction, or volume fraction), you must specify the following flow properties:

- Total flow
- Total flow unit

If you enter your component amounts as fractions, then you must also enter a total flow rate. If you enter composition amounts using quantitative flow units, CHEMCAD calculates the total flow rate for you.

Specifying Equipment Parameters

Once you have specified the necessary stream properties for your simulation, the next step is to enter specifications for the UnitOps. You can edit the properties of a UnitOp using any of the following methods:

- Double-click the UnitOp icon on the flowsheet.
- Click the UnitOp icon and then select **Specifications** > **Edit UnitOps** > **Select UnitOps**.
- On the **Simulation** tab in the CHEMCAD Explorer, expand **Flowsheet** and then **UnitOps**, right-click the UnitOp in question, and select **Edit UnitOp Data**.

The dialog box that displays when you go to edit a UnitOp's properties will depend on the type of UnitOp. The Stream Mixer UnitOp, for example, has only one specification that you can set, while the SCDS Column UnitOp has five tabbed pages of detailed settings.

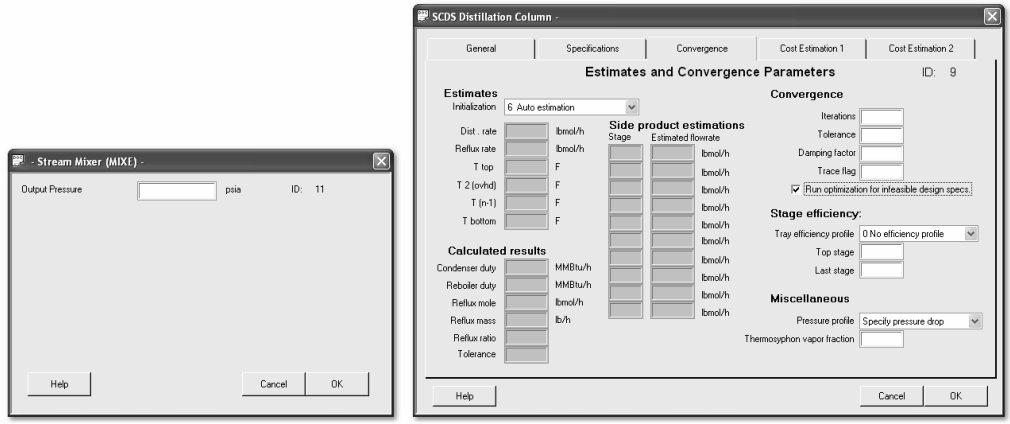


Figure 5-09: Two different UnitOps that require very different amounts of input

The detailed information about the specifications for each type of UnitOp is contained in the CHEMCAD Help system, which you can access from any CHEMCAD screen by pressing the **[F1]** key.

These specification screens do, however, have certain rules in common:

- Items with green text labels are required entries.
- All other entries are optional.
- Clicking **OK** saves your specification changes; clicking **Cancel** discards them.

After you click OK, CHEMCAD checks your data for internal consistency and then returns errors or warnings as warranted. These items display in the Messages pane in the CHEMCAD window.

Running the Simulation

Now that you've drawn the flowsheet and added detail to the streams and UnitOps that make up the flowsheet, you can run the simulation. You can either select **Run** > **Run** > **Run All** or simply click the **Run** button on the toolbar.

When you run a simulation, CHEMCAD calculates material and energy balances throughout the entire flowsheet and returns any errors or warnings discovered in the flowsheet. If the run completes successfully, a *Run finished* message appears at the far left of the status bar, at the very bottom of the CHEMCAD window.

Note: For preliminary checks of individual UnitOps or groups of UnitOps, you can select **Run** > **Run** > **Run Selected UnitOp(s)**.

Reviewing the Results

After a simulation has run, you can call up any number of individual text-based reports or graphical plots, either for on-screen viewing or for printing. Reports can provide data on any single stream or UnitOp, or any group of streams or UnitOps, in a steady-state or dynamic simulation. You can also request a consolidated report that provides comprehensive data on the streams and UnitOps you select.

Note: CHEMCAD reports, plotting, and plot printing are covered in detail in Chapter 8, *Output and Reports*.

Chapter 6

Using CHEMCAD for High-fidelity Modeling

Unit operation specifications in CHEMCAD vary greatly in detail, from vague and conceptual to extremely specific and realistic. Depending on the demands of your process and what you're trying to achieve with your simulation, you may work with what we call *low-fidelity modeling*, *high-fidelity modeling*, or both.

This chapter addresses CHEMCAD's capacity for high-fidelity modeling and how to achieve a high level of realism with your UnitOps.

What is high-fidelity modeling?

With low-fidelity modeling, you specify what you want, or what you have observed, and CHEMCAD makes its calculations based on the assumption that you can achieve what you've specified. It's common to specify observed properties such as temperature and/or pressure coming out of a UnitOp, or component purity coming out of a separation unit. Specifying temperature coming out of a heat exchanger is an example of low-fidelity modeling.

High-fidelity modeling, on the other hand, requires that you enter numerous extensive variables. CHEMCAD calculates the resulting conditions based on these detailed entries. With high-fidelity modeling, you're often required to specify geometry-related variables for a UnitOp so that CHEMCAD can calculate precise conditions at the equipment's outlet.

Here's the key distinction between low-fidelity and high-fidelity modeling in CHEMCAD:

- **Low-fidelity:** You specify the desired results and CHEMCAD assumes that you can achieve those results with the equipment you have.

- **High-fidelity:** You specify energy and equipment parameters and CHEMCAD calculates the actual results.

Criteria for High-fidelity Modeling

To take advantage of CHEMCAD's high-fidelity modeling capabilities, you must provide detailed specifications for your equipment. To do this, most UnitOps require that you select a calculation *mode* that allows for entry of high-fidelity-caliber detail.

For example, if you have a pump that is set to the default mode of *Specify outlet pressure*, you'll get a low-fidelity result from this pump—that is, the simulation will use the outlet pressure that you specify, but without consideration for the size of the pump, the amount of fluid entering the pump, or inlet pressure.

If you switch the pump to *Specify performance curve*, a high-fidelity mode, you'll need to enter data points from the pump's performance curve, either for a single speed line or for multiple speed lines. Using this mode, CHEMCAD will calculate the change of pressure head based on the performance data and the inlet volumetric flow rate. This provides a realistic pressure increase for the actual pump that your process uses.

Not every type of CHEMCAD UnitOp lends itself to high-fidelity modeling. The following sections discuss various types of UnitOps that do offer high-fidelity calculation modes, and provide some basic information about how to use those modes.

Introduction to Equipment Sizing

Equipment sizing in CHEMCAD is optional. It entails using the **Sizing** menu options, generally after running a simulation, to calculate approximate sizes for pipes, vessels, valves, orifices, and other equipment.

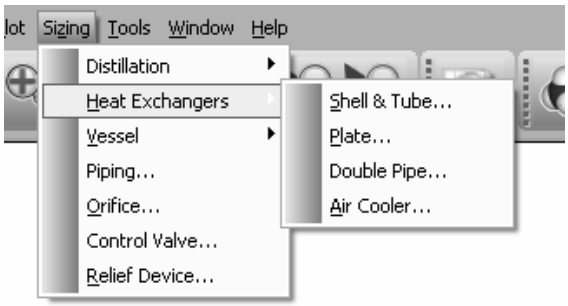


Figure 6-01: The Sizing menu, showing heat exchanger sizing options

Equipment sizing can complement low-fidelity results, and often provides an excellent starting point for high-fidelity modeling. You can use certain sizing results as input for high-fidelity models of UnitOps in your simulation. Specifying geometric parameters for UnitOps can help you obtain more realistic results.

Note that for low-fidelity modeling, sizing does not change converged flowsheet results. Also, for some UnitOps, certain geometry parameters must be entered regardless of the selected calculation mode.

High-fidelity Modeling and Sizing for Common UnitOps

High-fidelity modeling does not apply to all CHEMCAD UnitOps. This section summarizes those UnitOps for which you can use high-fidelity modeling, and compares that approach for each UnitOp type to low-fidelity modeling. Where applicable, UnitOp sizing is also discussed as it relates to low-fidelity versus high-fidelity modeling of these UnitOp types.

Piping

You can use either low- or high-fidelity modeling for piping in your simulation. Pipeline sizing is done based on the composition of a selected stream.

Low-fidelity

For low-fidelity modeling of piping, you are required to specify pipe diameter and length in most modes; design modes that calculate diameter are the obvious exception to this. The pressure drop through the pipe is calculated based on diameter, length, and flow rate through the pipe.

Sizing

To perform sizing calculations, select **Sizing** > **Piping**. Select one or more streams, then in the Pipe Sizing dialog box, select a sizing option and click **OK** for line sizing results. You can use these results, such as suggested pipe thickness and diameter, to specify geometry for a Pipe UnitOp, or simply review them for the information you need.

Line Sizing for Stream 1

Stream Properties:

- - Overall - -	
Mass flow lb/h	63329.1289
Actual dens lb/ft3	65.2969
- - Liquid only - -	
Mass flow lb/h	63329.1289
Actual dens lb/ft3	65.2969
Visc cP	1.1823

Pipe Parameters:

	Calculated	Next larger	Next smaller
Schedule	40	40	40
Flow Regime	Single phase	Single phase	Single phase
Pipe ID in	3.0680	4.0533	2.1316
Nominal Dia. in	3.0000	4.0000	2.0000
- - Overall - -			
Press Drop psi/100ft	1.5583	0.3898	9.7930
Velocity ft/sec	5.2447	3.0048	10.8651
- - Liquid only - -			
Reynolds Number	110272.1	83466.6	158716.8
Friction Factor	0.0205	0.0207	0.0209
Press Drop psi/100ft	1.5583	0.3898	9.7930

Line Sizing for Stream 2

Stream Properties:

- - Overall - -	
Mass flow lb/h	63329.1289
Actual dens lb/ft3	65.2969
- - Liquid only - -	
Mass flow lb/h	63329.1289
Actual dens lb/ft3	65.2969

Figure 6-02: Line sizing results from the Pipe Sizing dialog box

High-fidelity

In high-fidelity piping models, Pipe UnitOps interact with Node UnitOps to balance pressure and flow rates hydraulically among connected pieces of flow-based

equipment. Nodes must be placed on both sides of all Pipe UnitOps to be included in hydraulic balance; pressure and flow constraints are set at the nodes, not in the pipes.

A high-fidelity piping model can show changes in flow rate based on back pressure where two pipes mix, whereas a low-fidelity model would simply assign the lower of two specified pressures to the outlet without consideration for back pressure.

Pumps, Compressors, and Expanders

You can create pump, compressor, and expander UnitOps using either low-fidelity or high-fidelity modeling.

Low-fidelity

For these equipment types, CHEMCAD calculates power usage and thermal effects on the fluid, based on specified output pressure or pressure increase. Other parameters, such as efficiency, are optional but do affect results.

High-fidelity

To produce a high-fidelity model for these equipment types, you must select the operation mode in which you specify performance curves—that is, pressure change as a function of volumetric flow rate. This performance information is generally available from the equipment vendor. Based on the volumetric flow entering the UnitOp, CHEMCAD calculates outlet pressure.

As with piping, high-fidelity modeling for pumps, compressors, and expanders can be used with nodes as part of a hydraulic flow balanced network.

Vessels and Tanks

You can add vessels and tanks to your simulations using high-fidelity modeling, or perform limited approximation of these equipment types with low fidelity in steady state. Sizing is available for certain types of vessels.

Low-fidelity

With low-fidelity modeling of a vessel or tank, a stream enters the Flash UnitOp and separates into vapor and liquid; CHEMCAD does not consider hold-up or liquid level in the tank. If you want to take a steady-state snapshot of the vessel, you can manually adjust the flow rate and/or thermal conditions to make volumetric flow rates match the volume of the vessel.

Note: The Tank UnitOp is specifically intended for use with the Batch Column UnitOp. It does not represent a standard storage tank for general purposes.

Sizing

To calculate sizing for a vessel, select a Flash UnitOp and then select **Sizing** > **Vessel**. Choose either **LV Vessel** (liquid-vapor vessel) or **LLV Vessel** (liquid-liquid-vapor vessel), depending on your needs. In the resulting dialog boxes, enter the appropriate values for your vessel and click **OK**.

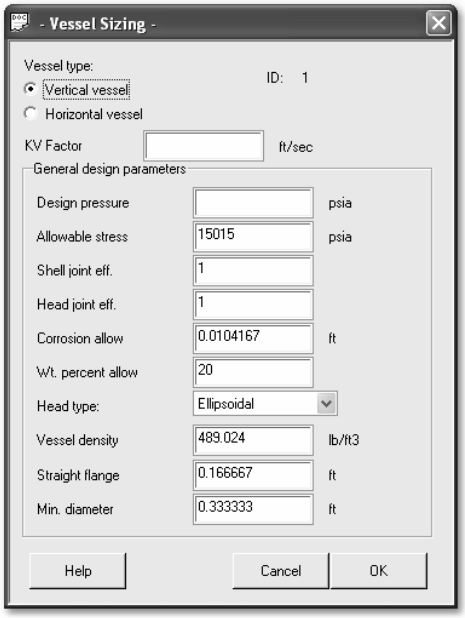


Figure 6-03: Sizing a vessel in CHEMCAD

The results that CHEMCAD returns include basic vessel geometry such as height and diameter.

You can also perform vessel sizing on a converged distillation column to calculate geometry for a reflux drum or similar piece of equipment.

High-fidelity

You can perform high-fidelity modeling only on batch reactors and dynamic vessels, and only with a CC-DYNAMICS license (for dynamic vessels, a CC-SAFETY NET license will suffice). If you specify the geometry of your vessel and use CHEMCAD's dynamics mode, you can study what happens in the vessel over time as material is added or withdrawn.

Unlike simple flash vessels, batch reactors and dynamic vessels do consider hold-up, liquid level, and variable pressure over time.

Valves

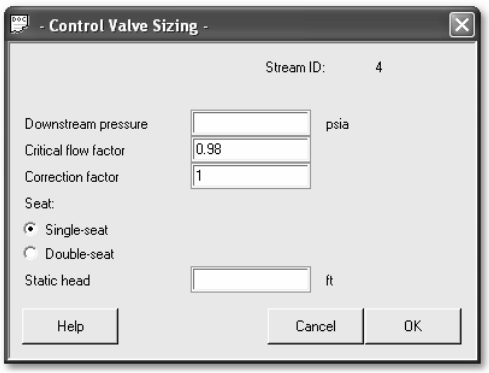
Valve modeling in CHEMCAD can be either low-fidelity or high-fidelity. You can size a control valve based on any flowsheet stream.

Low-fidelity

The VALV UnitOp is used for low-fidelity modeling of a valve. For this type of UnitOp, you specify outlet pressure or pressure decrease through the valve.

Sizing

Select **Sizing** > **Control Valve**, then select a stream. In the Control Valve Sizing dialog box, specify the outlet pressure for the theoretical valve, and enter other specifications as appropriate. When you click **OK**, CHEMCAD returns information such as capacity coefficient (Cv) and valve size.



High-fidelity

The CVAL UnitOp is used for high-fidelity valve modeling. Decide which values you will provide and which values CHEMCAD will calculate, and select the appropriate operating mode in the Control Valve dialog box. Provide the valve's Cv value, and any other specifications as needed.

Control valves can be used with nodes as part of a hydraulic flow balanced network.

Columns

Columns in CHEMCAD can be modeled as either low-fidelity or high-fidelity. You can perform sizing on any converged column.

Low-fidelity

For low-fidelity modeling of columns, use the Tower, Tower Plus, or SCDS UnitOps. Specify ideal stages and the conditions at the reboiler and condenser, as applicable. A low-fidelity column model does not consider mass transfer effects or column internals.

Different column specifications can provide more realism without taking geometry into account. Specifying top purity is a very low-fidelity model, while specifying reflux ratio or condenser duty can bring your results closer to reality.

Sizing

After running your simulation, click the UnitOp representing the distillation column and select **Sizing** > **Distillation**; choose either **Trays** or **Packing**, based on the type of column.

The resulting dialog boxes prompt you to enter information about your trays or packing and the calculation methods you want to use for column sizing. You will

generally need to enter some geometry and hydraulic parameters to complete column sizing.

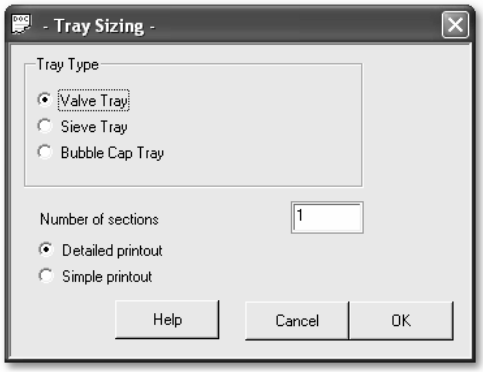


Figure 6-04: Specifying high-level tray data for distillation column sizing

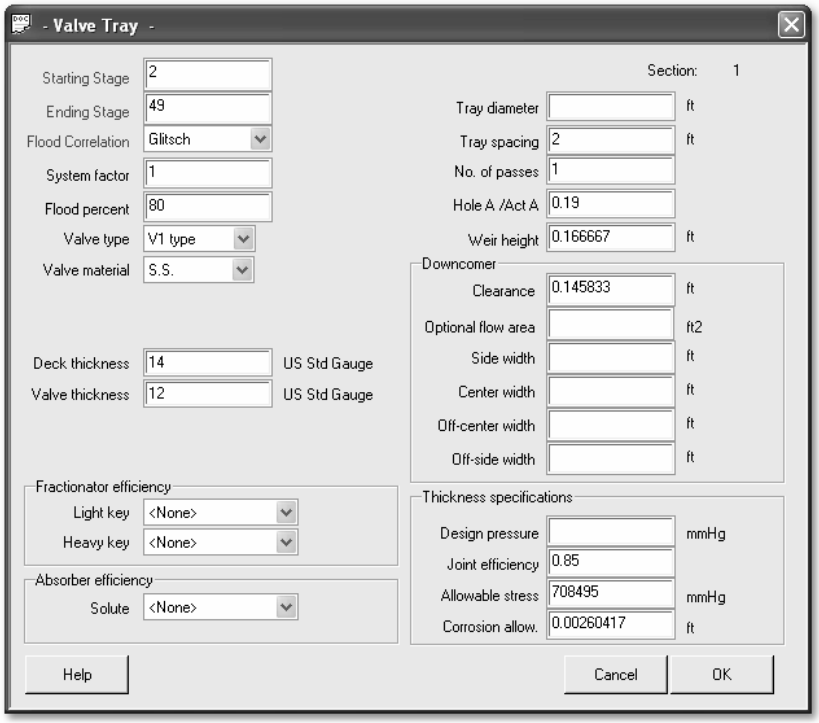


Figure 6-05: Specifying detailed tray data

Based on flowsheet values and your sizing input, CHEMCAD returns column geometry information such as height and diameter. It also provides hydraulic performance information such as predicted amount of flooding.

Note: The results of column sizing calculations *do not* interactively change the results of the flowsheet simulation.

High-fidelity

To perform high-fidelity modeling of a distillation column in steady state, use the SCDS UnitOp and select either of the mass-transfer simulation models for the column.

You will need to specify geometry for the column and choose a calculation method for the selected mass-transfer model. CHEMCAD calculates column performance based on your packing or tray specifications.

For columns, mass-transfer-based modeling performs rigorous non-equilibrium mixing of vapor and liquid, whereas low-fidelity modeling assumes ideal mixing.

To perform high-fidelity modeling of a distillation column in dynamics, specify the geometry of the column and details about the control system. This dynamic distillation can consider column hold-up and the effect of variables changing over time.

Note: The Shortcut Column UnitOp is *not* a rigorous calculation model. Unless your system satisfies the constant molar underflow assumption, you should consider using a different type of distillation column.

Heat Exchangers

When specifying a heat exchanger in a simulation, you can use either low- or high-fidelity modeling as well as sizing, depending on the type of heat exchanger involved.

Low-fidelity

When creating a simulation, you can use a low-fidelity approach by simply specifying the thermal conditions coming out of the exchanger. Specifying heat duty instead of merely an outlet temperature brings your results closer to reality, but this approach still doesn't consider geometry.

Sizing

You can use the CC-THERM module for rigorous calculation of heat transfer coefficient (U) based on heat exchanger geometry. In rating mode, CC-THERM determines whether the user-specified heat exchanger is capable of the flowsheet heat exchanger performance. In design mode, CC-THERM calculates an exchanger design that is capable of the flowsheet performance.

High-fidelity

For some exchanger categories—specifically shell-and-tube and double-pipe—you can use the rigorous CC-THERM model to calculate heat exchanger performance. The flowsheet results are based on rigorously calculated U value and the specified exchanger geometry. You can also determine approximate fouling of a unit if actual outlet temperatures are known.

Summary

Geometry Data			Heat Transfer Data		
Exchanger Class		R	Effective Transfer Area	ft2	5390.52
Exchanger Type		AEL	Area Required	ft2	3687.47
Shell I.D.	ft	3.33	Excess %		46.18
Shell in Series		1	COR LMTD	F	27.36
Shell in Parallel		1	Overall Coefficient (Calculated)	Btu/hr-ft2-F	27.51
Number of Tubes		1396	Overall Coefficient (Service)	Btu/hr-ft2-F	18.82
Tube Length	ft	20.00	Heat Calculated	MMBtu/h	4.06
Tube I.D.	ft	0.05	Heat Specified	MMBtu/h	2.78
Tube O.D.	ft	0.06	Shell Side Film Coefficient	Btu/hr-ft2-F	89.63
Tube Pattern		TRI60	Tube Side Film Coefficient	Btu/hr-ft2-F	53.10
Tube Pitch	ft	0.08	Shell Side Fouling	hr-ft2-F/Btu	1.0000E-03
Number of Tube Passes		1	Tube Side Fouling	hr-ft2-F/Btu	1.0000E-03
Number of Baffles		8	Tube Wall Resistance	hr-ft2-F/Btu	1.9829E-04
Baffle Center Spacing	ft	2.0000	Fin Resistance	hr-ft2-F/Btu	
Baffle Cut (area %)		32			
Baffle Type		SSEG			
			Thermodynamics and Others		
			K model		Peng-Robinson
Fluid Dynamics Data			H model		Peng-Robinson
Shell Side Pressure Drop	psi	10.2335	Data Source		Library
Tube Side Pressure Drop	psi	4.6942	Number of Components		9
Average Shell Side Velocity	ft/sec	16.30	Calculation Mode		Rating
Average Tube Side Velocity	ft/sec	13.48			

Warning in Geometry->baffle: Inlet baffle spacing outside of TEMA standard RCB 4.5, 8 - 29.937 inch.
Warning in Geometry->baffle: Outlet baffle spacing outside of TEMA standard RCB 4.5, 8 - 29.937 inch.

Figure 6-06: Heat exchanger summary report generated as an Excel worksheet

Relief Devices

For relief devices, sizing is not necessarily distinct from low-fidelity modeling. To model dynamic relief of a vessel, you can instead use high-fidelity modeling.

Low-fidelity

To model a steady-state snapshot of a relief device, select **Sizing** > **Relief Device**, specify rating or design mode, and select the appropriate options for your relief scenario. When you click **OK**, CHEMCAD returns a relief device calculation summary.

If you select the *Rigorous integral analysis* design method when sizing a relief device, you will obtain a more dynamic result.

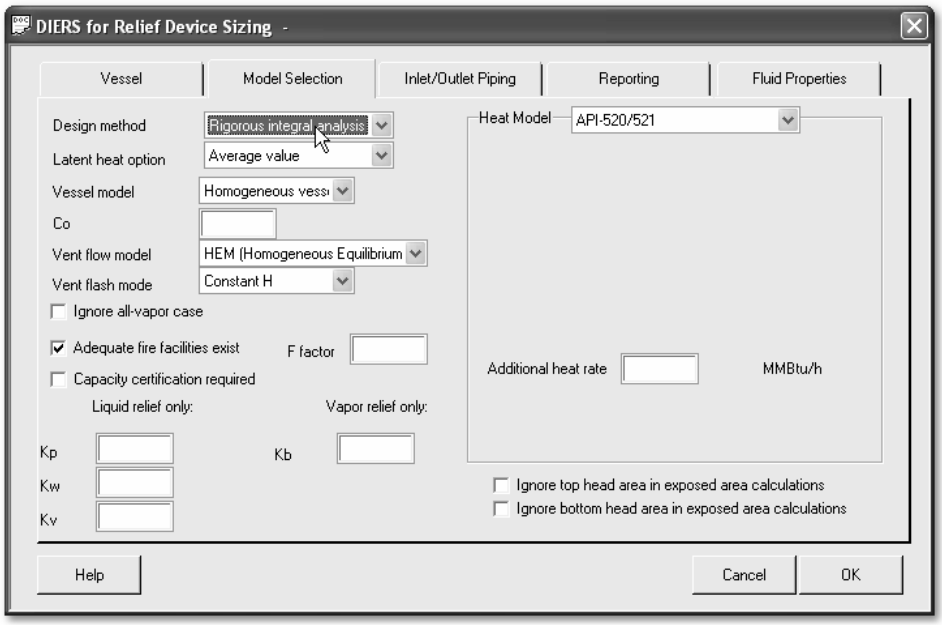


Figure 6-07: Selecting the rigorous integral analysis method for relief device design

High-fidelity

You can perform high-fidelity relief device modeling for the Batch Reactor and Dynamic Vessel UnitOps. You can specify the relief device nozzle area, as well as other specifications for your relief scenario. This enables you to study the dynamic relief of the vessel.

Licensing Considerations for High-fidelity Modeling

To use the heat exchanger sizing functionality, you must currently have a valid license for the CC-THERM module of CHEMCAD. To use batch reactors, you'll need a valid license for the CC-DYNAMICS module. For dynamic vessels, a license for either CC-DYNAMICS or CC-SAFETY NET is required.

If you don't currently have access to the heat exchanger sizing or dynamics features and want to add any of these modules to your copy of CHEMCAD, contact the person within your organization who handles software licensing, or if appropriate, you can contact Chemstations or a CHEMCAD distributor directly. For a complete list of Chemstations contacts for all parts of the globe, see our web site (www.chemstations.net/contact.htm).

License Settings

If you've just added modules to your CHEMCAD license, you should return to the License Settings screen to change settings before proceeding.

Select **Tools** > **Options** > **License Settings** (if a simulation is open) or **License** > **License Settings** (if no simulation is open) to bring up the License Settings screen. Move the slider for each newly-installed module to **As Needed** and then click **OK** to apply your changes.

You may see a Trace Messages window; if one appears, click **OK** to close it. The next screen that appears is the Licenses in Use screen, where you can review the list of CHEMCAD products for which you currently have licenses. Click **OK** to close this screen and return to the main CHEMCAD window.

Chapter 7

Building and Using a Dynamic Simulation

While steady-state modeling can provide all of the information you need for many purposes, it's often informative to look closely at the changes over time that affect your streams and equipment. CHEMCAD's CC-DYNAMICS module makes it possible to simulate a process over time.

What do we mean by dynamics?

We use the term *dynamics* to describe modeling a chemical process over a set period of time. During the course of a real-world chemical process, factors such as utility temperature, feed composition, and liquid levels tend to change. Modeling the response of your process to these changes can help you understand and predict what might happen with your process over time.

Given a flowsheet, a length of time to run, and the calculation interval to use, CHEMCAD can return detailed results that take into account these types of changes. The program can consider the material holdup within process equipment such as tanks, reactors, and pipes. It also enables you to model control systems such as PID controllers.

Licensing Considerations

To use the functionality described in this chapter, you must have a valid license for the CC-DYNAMICS module of CHEMCAD.

If you don't currently have access to the dynamics features and want to add CC-DYNAMICS to your copy of CHEMCAD, contact the person within your organization who handles software licensing, or if appropriate, you can contact Chemstations or a CHEMCAD distributor directly. For a complete list of

Chemstations contacts and CHEMCAD distributors for all parts of the globe, see our web site (www.chemstations.com/contact.htm).

License Settings

If you've just added CC-DYNAMICS to your CHEMCAD license, you'll need to return to the License Settings screen to change a setting before you can run dynamic simulations.

Select **Tools** > **Options** > **License Settings** (if a simulation is open) or **License** > **License Settings** (if no simulation is open) to bring up the License Settings screen. Move the slider for CC-DYNAMICS to **As Needed** and then click **OK** to apply your change.

You may see a Trace Messages window; if one appears, click **OK** to close it. The next screen that appears is the Licenses in Use screen, where you can review the CHEMCAD products (including CC-DYNAMICS) for which you currently have licenses. Click **OK** to close this screen and return to the main CHEMCAD window.

Additional Input for Dynamic Operation

Before you create a dynamic simulation, you'll need to gather the relevant information about your UnitOps and streams, as you would with any simulation. In addition, you need to be able to answer the following dynamics-specific questions:

- How long will the simulation run?
- What will be the interval (delta time/step size) between calculations?
- What is the change that you want to study over time?
- If applicable, what is the initial composition and charge of any dynamic vessels or batch reactors?

The basic steps for a dynamic simulation are largely the same as those for a steady-state simulation, with a few vital differences:

1. Create a new simulation.
2. Select engineering units.
3. Draw the flowsheet.
4. Select components.
5. Select thermodynamics options.
6. Specify feed streams and initial stream conditions.
7. Set specifications for UnitOps.
8. Run the simulation in steady state to obtain time-zero values.
9. Switch the simulation to dynamics.
10. Specify dynamics settings, such as run time and initial charge(s).

11. Run the simulation in dynamics.
12. Review the results.
13. Re-run or extend the simulation as needed.
14. Generate plots and reports as needed.

Before you start working on a dynamic simulation, it's important to have as much information about your process as possible, a clear idea of what you want to find out, and a strategy for producing the results you need.

Strategies for Dynamic Simulations

When you start planning a dynamic simulation, it's vital that you know what question or questions you are trying to answer. To get useful, informative results, you should start with a simple question and then refine the simulation and run it again.

For example, to discover how heat affects a vessel's temperature over time, you might start by applying constant heat to the vessel for the duration of your dynamic simulation. You can then save a copy of that simulation, change it to use variable heat, and review the results to see how they differ from the original. Based on that second simulation, you can make another copy, and this time try variable heat with a control system to attempt to maintain a consistent temperature. Each of these dynamic simulations would bring you closer to what you actually want to discover. Each subsequent simulation requires more information from you to run and return the results you want.

While there is no requirement that you approach dynamics problems this way, it's a sound practice that will save you time and frustration in the long run.

Setting Up Dynamic Operation

Before you can run a dynamic simulation, you need to provide parameters such as run time and step size. First, however, you must activate CHEMCAD's dynamics mode.

Switching to Dynamics

Follow these steps to switch a simulation from steady-state to dynamic operation:

1. Open the simulation and select **Run** > **Convergence**. This brings up the Convergence Parameters dialog box.
2. In the lower right portion of the dialog box, click in the **Steady State/Dynamics** field and select **Dynamics**.

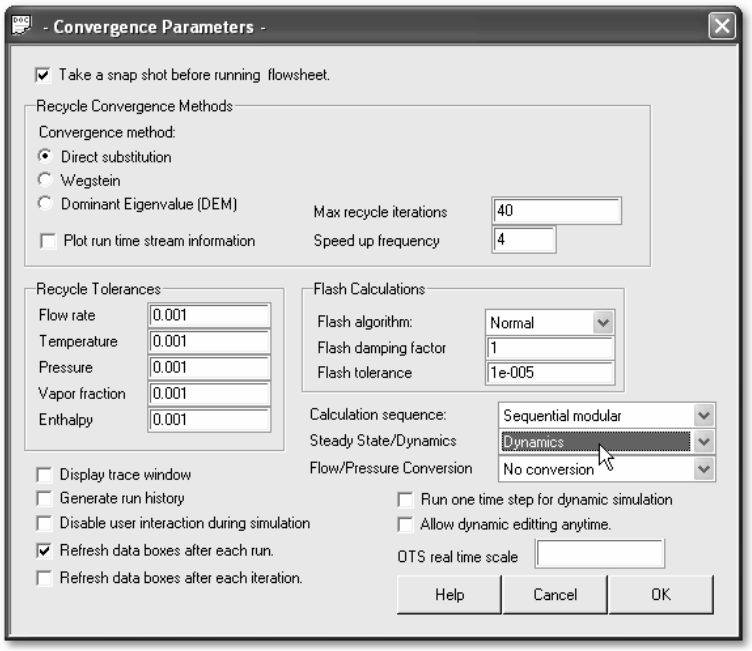


Figure 7-01: Switching to dynamics

3. Click **OK** to save the changes and close the dialog box.

After you switch to dynamics, you'll notice that a few things have changed on the CHEMCAD screen:

- The status bar at the bottom of the main CHEMCAD window changes. A few inches from the right edge of the screen, instead of the words *Steady State*, you'll now see *DTime* and a time counter displaying the number of minutes your simulation has run. Before you run the simulation, the *DTime* setting displays **0:00 min**.
- The steady-state **Run All** button on the toolbar is disabled, and the dynamics buttons are now activated. These buttons, shown in Figure 7-02, are (left to right) **Set Run Time**, **Reset to Initial State**, **Run Dynamic Simulation**, **Plot Dyn Streams**, and **Plot Dyn UnitOps**.

Figure 7-02: Toolbar buttons for dynamics

- You can now select **Run** > **Dynamics** to bring up the Dynamics Menu. This window provides convenient access to all dynamics settings and commands.

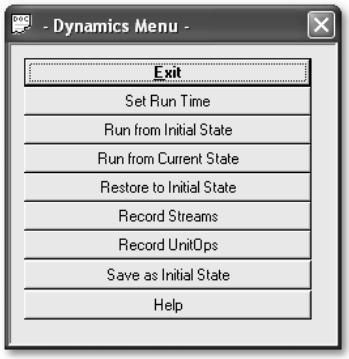


Figure 7-03: The Dynamics Menu

Setting the Run Time

The next step is to set the run time for the simulation. First decide whether your run will require a single step or multiple steps.

A step in this case refers to a time period during which CHEMCAD will capture data from the simulation at uniform intervals. For example, you might set up a single-step dynamic run of 60 minutes, with a step size of one minute, for a total of 60 data points for the run. If this is all that you need to do, your run can be accomplished in a single step.

If, on the other hand, you need to run your process for 60 minutes capturing data at one-minute intervals, and then switch to capturing data every 30 seconds for the next 20 minutes, you'll need to use two steps. If you want to record data every five minutes for the first hour, every minute for the second hour, and every 30 seconds for the third hour, you'll need to use three steps.

The step size that you select will have an impact on the accuracy of the results and the speed of the calculation. Smaller time steps produce more precise results, but also require more time to make the run. Smaller isn't always better, however, as extremely small time steps can lead to significant round-off error.

Once you know how many steps you need to use and what your data-capture interval will be for each step, follow these steps to set the run time parameters:

1. Click **Set Run Time** on the Dynamics Menu, or click the **Set Run Time** button on the toolbar. This brings up the Dynamic Run Time Schedule dialog box.

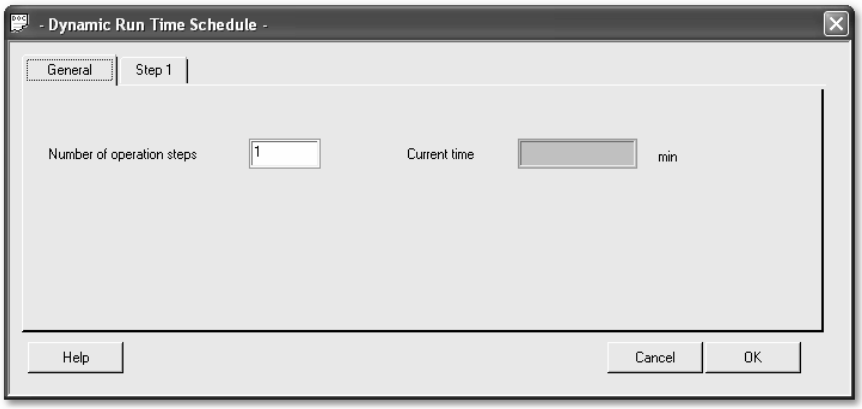


Figure 7-04: The General tab on the Dynamic Run Time Schedule dialog box

2. On the **General** tab, set the number of operation steps you plan to use, or leave the default setting of **1**. The maximum number of steps that you can specify is 10.

Note: When you initially set up dynamics for a simulation, the **Current time** display field on this tab will be empty. After the simulation has run, this field displays the total time of a completed run or the current time of an interrupted run.

3. Now click the **Step 1** tab and specify the parameters for this portion of the dynamic run. Enter the total time for this dynamic step in the **Run time** field, and the interval in minutes in the **Step size** field.

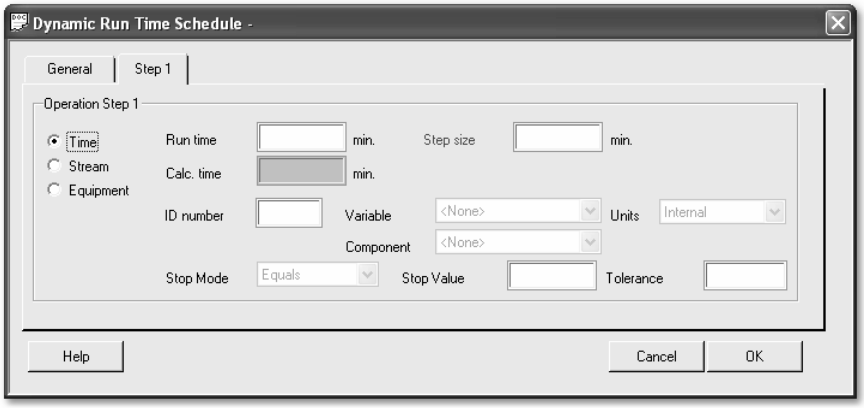


Figure 7-05: The Step 1 tab on the Dynamic Run Time Schedule dialog box

4. If you have other steps to specify, click each tab in turn and enter the **Run time** and **Step size** information.

5. When you have specified all steps, click **OK** to return to the main CHEMCAD window.

The Dynamic Run Time Schedule dialog box also allows for conditions other than time to determine the duration of a dynamic operation step. If you select **Stream** or **Equipment** instead of the default **Time** option, you can specify a stream or UnitOp parameter that will trigger the end of this step, if that parameter is reached before the step's run time is up.

Selecting Streams and UnitOps

Now that you have specified how long your dynamic process will run, you need to tell CHEMCAD what stream and UnitOp data to record during the run.

1. If the Dynamics Menu is not already open, select **Run** > **Dynamics** to open it, then click the **Record Streams** button.
2. In the Record Streams dialog box, do one of the following:
   - Check the **Select streams from flowsheet** box, click **OK,** and then use the mouse to add streams to the Select Streams dialog box.
   - Type the names of streams you want to record in the **ID** boxes.

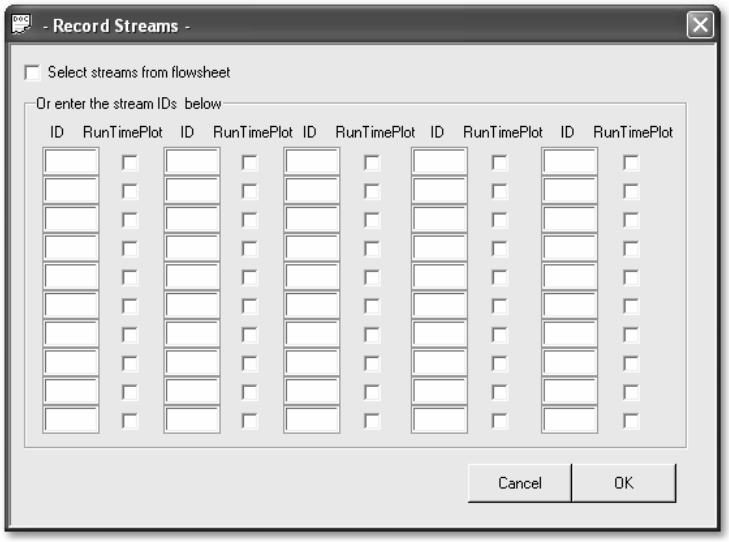


Figure 7-06: The Record Streams dialog box

3. When you have selected all the streams you want to record, click **OK** to return to the Dynamics Menu.
4. Now click the **Record UnitOps** button. In the Record UnitOps dialog box, select UnitOps in the same way that you selected streams in step 2.
5. Click **OK** to return to the Dynamics Menu.

Note: In both the Record Streams and Record UnitOps dialog boxes, you can use the **RunTimePlot** check boxes to include selected items in a real-time plot. Selecting items for runtime plotting leads to another dialog box (either Dynamic Stream Plot Options or Dynamic Equipment Plot Options), where you can select plot specifics for each stream or UnitOp. It is recommended that you use runtime plotting in moderation, as too many streams and UnitOps can become visually confusing and slow down calculations considerably.

Running a Dynamic Simulation

Now that you have set the run time and recording parameters, you can run the simulation. When you run a dynamic simulation in CHEMCAD, a calculation of the entire flowsheet runs for each step in the time range that you select.

In dynamics mode, you have three options for running a simulation: run from the simulation's initial state, run from the simulation's current state, or advance the simulation one time interval at a time manually.

Note: At any point during a dynamic run, you can press the **[ESC]** key on your keyboard to stop the run after the current calculation. When you do this, you will see a *Program interrupted* message. Click **OK** to close the message box, and then either inspect your run results or select a run command to continue.

Run from Initial State

This option resets the flowsheet to its initial conditions and begins the dynamic simulation. When you run a simulation this way, all results from previous simulations are discarded.

To use this option, use either the **Run from Initial State** button on the Dynamics Menu or the **Run Dynamic Simulation** button on the CHEMCAD toolbar.

Run from Current State

When you use this option, the dynamic run begins from the current conditions. Those conditions might be the initial state of the flowsheet, the end of a previous run, or the middle of an interrupted run. Selecting this option continues the simulation from the current state, i.e., from the last calculated result.

You can use this option only when some calculations remain to be run. This means that unless you have interrupted the run using **[ESC]** or the step-by-step method described in the next section, you must schedule one or more additional steps using the **Dynamic Run Time Schedule** before continuing.

Use the **Run from Current State** button on the Dynamics Menu to run the simulation starting from current conditions.

Run One Step at a Time

If you want to get a detailed view of your dynamic run as it unfolds, you can choose to run one interval at a time. With this option, the dynamic run will stop after each discrete time step. To run the next time step, you will need to use the **Run Dynamic Simulation** toolbar button or the **Run from Current State** button on the Dynamics Menu.

To use this frame-by-frame approach to dynamics, select **Run** > **Convergence** and then check the box called **Run one time step for dynamic simulation**. Click **OK** to confirm this change. To turn off this feature, return to the Convergence Parameters dialog box to clear this check box.

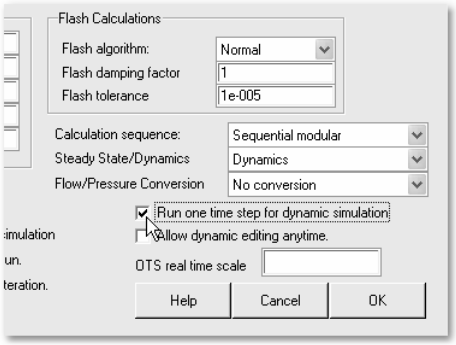


Figure 7-07: Convergence Parameters setting to run one step at a time

Other Dynamic Commands

In addition to the options for dynamic run setup and dynamic commands, the Dynamics Menu offers two other items: **Reset to Initial State** and **Save as Initial State**.

Reset to Initial State

In a dynamic simulation, you can change stream and UnitOp specifications only when the dynamic time is set to zero. During or after a run, if you attempt to edit the specification dialog box for a UnitOp, you will find the **OK** button disabled and a message instructing you to restore the simulation to its initial state.

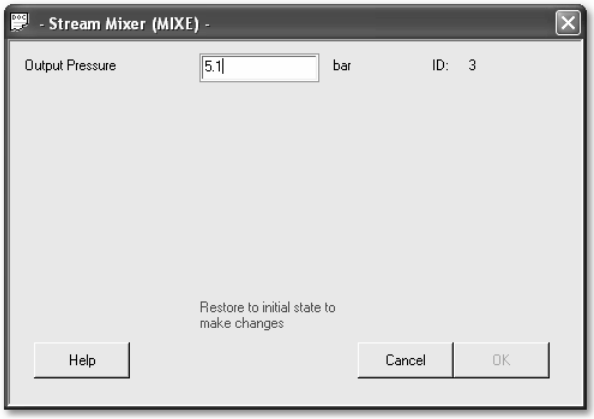


Figure 7-08: A UnitOp specification dialog box during a dynamic run

To return the simulation to its initial state—also known as *time zero*—click the **Reset to Initial State** button on the Dynamics Menu, or use the **Reset to Initial State** button on the main CHEMCAD toolbar.

Note: An advanced feature to allow specification editing at any time is available, but should be used with extreme caution to avoid confusion and unintended results. This feature is controlled by a check box on the Convergence Parameters dialog box.

Save As Initial State

The **Save as Initial State** command sets the current conditions of the dynamic run as the new initial state. It discards all parameters from the previous initial state, and makes it impossible to recover the previous initial state data.

An example of a dynamic run can illustrate the usefulness of this command. Suppose that you run a simulation for five minutes and the temperature in a vessel increases from 50° C to 70° C. You decide that 70° C is a better starting point for this vessel, and you want to capture all of the other values that correspond to that temperature in this vessel. You can achieve this by saving the current conditions as the initial state.

To do this, click the **Save as Initial State** button on the Dynamics Menu. You will see a message warning you that you will lose the original state conditions if you continue. If you are prepared to do this, click **Yes**. For our example, this would mean losing the first five minutes of your previous run, along with the 50° C starting temperature for the vessel.

After you save a new initial state, the **Run from Initial State** and **Reset to Initial State** commands both reference your new initial state settings.

Output from Dynamic Simulations

The results from dynamic simulations are markedly different from those produced by steady-state simulations, primarily in that they record data trends over time instead of a static snapshot of a fixed process. With dynamic simulations, comparisons of slightly different process specifications, and of the same process at different points during a run, can be very useful.

For this reason, you may find that graphical reports provide the most useful information when you're working with dynamic simulations. CHEMCAD provides a series of dynamics plotting options to meet this need; you can also generate various text-based reports, and view calculated flowsheet values at any point during a dynamic run or after a run is complete.

Reviewing the Flowsheet Specifications

A snapshot of flowsheet values from a dynamic run doesn't provide as much value as it would for a steady-state run, but it can come in handy in many situations.

After running a dynamic simulation, you can view the data behind any flowsheet stream or UnitOp to see the effects of the run calculations. Double-click any stream or UnitOp on the flowsheet to review its end-of-run values.

You can also stop to review flowsheet data in the middle of a run, either by using the **Run one time step for dynamic simulation** option or by pressing **[ESC]** to pause a run. Once the run has stopped, you can double-click any stream or UnitOp to review its current values.

Plotting Dynamic Results

You can plot the results of dynamic simulations using either the **Plot** menu or the dynamics buttons on the main CHEMCAD toolbar.

Dynamic plots display selected values over time. The following dynamic plots are available:

- **Batch Reactor/DVSL History:** This plot displays selected values for a batch reactor or dynamic vessel, including composition of the vessel contents over time. The dialog box used to generate this plot is user-friendly and focuses on the most commonly used variables for these types of equipment.
- **Dynamic Column History:** This plot displays selected values for a dynamic column, including composition of trays, distillate, and bottoms.
- **Dynamic Stream History:** This plot displays selected stream properties from any recorded stream. You can also generate this report using the **Plot Dyn Streams** toolbar button.
- **Dynamic UnitOp History:** This plot displays selected UnitOp parameters from any recorded UnitOp. You can also generate this report using the **Plot Dyn UnitOps** toolbar button.

Note: For the Dynamic Stream History and Dynamic UnitOp History plots, be sure to record the streams and UnitOps that you want to study. You can only request these plots for recorded streams or UnitOps.

Text-based Dynamic Reports

Based on the graphical results of your dynamic simulation run, you may decide to make changes to your process, run parameters, or both, and then re-run the simulation. When you have fine-tuned your simulation and obtained satisfactory results, you can view those results in text form as well as graphical form, for a more detailed look at exact values.

To access text-based dynamic reports, select **Report** > **Dynamics** and then select one of the following reports:

- **Dynamic Column History:** This report provides dynamic column results for a selected column. The Print Report Options dialog box offers the most relevant items for dynamic column reporting.

- **Dynamic Stream History**: This report provides stream histories for a specific stream that you select, based on the interval that you specify and including the compositions, components, and stream properties that you select.
- **Dynamic UnitOp History:** This report provides detailed information about a dynamic UnitOp in the simulation, based on the interval that you specify and including the UnitOp parameters that you select.

Note: For the Dynamic Stream History and Dynamic UnitOp History reports, be sure to record the streams and UnitOps that you want to study. You can only request these reports for recorded streams or UnitOps.

Chapter 8

Output and Reports

One of CHEMCAD's greatest strengths is its capacity to provide detailed, customized information about equipment, streams, and processes. You can create custom reports from simulations, spec sheets for UnitOps, and databoxes for process flow diagrams, and you can plot or print any of these items in the most appropriate format.

Text Reports

CHEMCAD can produce a wide array of customizable text-based simulation reports, based on stream data, UnitOp data, flowsheet data, or dynamics. If you prefer, you can produce one consolidated report incorporating all of the available text report data.

Report Setup

Before you run, view, or print reports, you should check the settings that determine which programs CHEMCAD will use to display and print your reports.

For individual text reports, you can choose to use either WordPad or Excel. By default, CHEMCAD uses WordPad. To switch to Excel, select **Tools** > **Options** > **Report Viewer Settings** and then check the box called *Use Microsoft Excel instead of WordPad*. Click **OK** to return to the main CHEMCAD workspace.

For the consolidated report, you can use either Word or Excel. To choose a program to display and print this report, select **Report** > **Consolidated Report**, then click **Report Format** at the top of the Consolidated Report menu. This brings up the Report Format dialog box. Choose whether you want your consolidated report

results to appear in a Word document or an Excel workbook file, and then click **OK** to apply your change.

Stream-based Reports

A number of CHEMCAD reports are available to analyze stream data from a simulation. To access any of the following reports, select the appropriate item from the **Report** menu. The results will display in either WordPad or Excel, depending on how you've configured CHEMCAD to handle text reports.

> **Note:** By default, these reports will use the engineering units you selected when building this simulation. You can, however, use different flow rate units when running reports. To change flow rate units for reporting, select **Report** > **Set Flow Units**. In the View Flow Rate Unit dialog box, select the units you want to use and then click **OK**. The next time you run stream composition or property reports, the units that you've selected here will be the default setting; you can change the flow rate units again as needed.

Stream Groups

For stream composition and property reports, you can create custom stream groups within a simulation to streamline your report requests.

For example, if you have a process that involves ten different feed streams, and you frequently run reports on this group of streams, you can set up a group consisting of just those streams. Then, whenever you want to obtain composition or property data for those streams, you're just a few clicks away anytime the simulation is open.

The quickest way to set up any group is to use the CHEMCAD Explorer. Follow these steps to create a stream group:

1. In the CHEMCAD Explorer pane, find the top-level item called Groups. Click the plus sign next to **Groups** to expand this item.

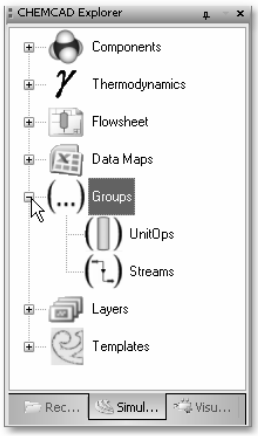


Figure 8-01: Expanding the Groups item in CHEMCAD Explorer

2. Now right-click the **Streams** item under Groups and select **New**.

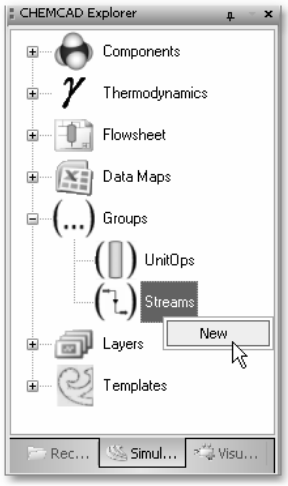


Figure 8-02: Creating a new stream group

3. In the New Group dialog box, replace the default name (such as **Group 1**) with a descriptive name for your group, then click **OK**.

Figure 8-03: Naming the new stream group

4. In the Edit Stream Group dialog box, select the streams for this group, either by typing in the stream numbers (one per line) or by clicking on streams in the flowsheet. Click **OK** to close the dialog box.

5. As soon as you finish creating the group, its name appears under Streams in the CHEMCAD Explorer. From here, you can right-click the group name and select any of the following:

   - **View/Edit:** Open the Edit Stream Group dialog box, where you can add or delete stream numbers to include in the group.
   - **Rename:** Open the Rename Group dialog box, where you can type a new name for the stream group.
   - **Copy:** Open the Copy Group dialog box, where you can type a new group name to make an exact copy of the stream group. After you click **OK**, you can then edit the new copy of the group to fit your needs.
   - **Delete:** Remove this stream group from the simulation. If you're sure about deleting the group, click **Yes** in the dialog box that appears.
   - **Composition:** Run an instant stream composition report for the streams in the group.

- **Properties:** Run an instant stream properties report for the streams in the group.

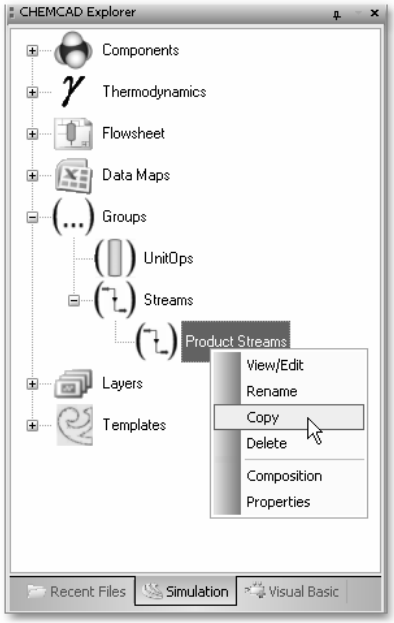


Figure 8-04: Right-click menu options for custom stream group

Note: The commands to create, edit, and remove stream groups are also offered on the **Report** menu, under both **Stream Compositions** and **Stream Properties**.

Stream Compositions

You can run a stream composition report based on all streams, or you can specify which streams to include. To run a stream composition report, select **Report** > **Stream Compositions** and then select from the following options:

- **Select Streams:** Choose the streams you want to include in the Select Streams dialog box, either by typing in the stream numbers (one per line) or by clicking on streams in the flowsheet. Click **OK** to close the dialog box and display the report.
- **All Streams:** This report displays all stream composition data for the entire flowsheet.
- **Feed Streams:** This report displays stream composition data only for streams issuing from a Feed icon on the flowsheet.
- **Product Streams:** This report displays stream composition data only for streams terminating in a Product icon on the flowsheet.

- **Unit Streams:** This report displays all inlet and outlet stream composition data for a specified UnitOp on the flowsheet. If no UnitOp icon is selected when you run the report, you'll see the Select UnitOps dialog box; type the UnitOp ID or click the UnitOp on the flowsheet and then click **OK** to display the data. If you select a UnitOp icon before running the report, the data will display without further input.

You can quickly display stream composition for a single stream at any time, simply by right-clicking the stream in the flowsheet and selecting **View Composition**.

Stream Properties

Before running reports on stream properties, you'll need to specify which properties to include. To do this, select **Report** > **Stream Properties** > **Select Properties**. This opens the View Property Options dialog box, where you can review which properties are currently selected.

If you want to add any properties, check the appropriate boxes; to remove properties, click on checked boxes to clear them. If applicable, click the **Crude/Solids** tab, and make any changes to the properties on that tab. Click **OK** to return to the main CHEMCAD window.

To run a stream properties report for the properties you've specified, select **Report** > **Stream Properties** and then select from the following options:

- **Select Streams:** Choose the streams you want to include in the Select Streams dialog box, either by typing in the stream numbers (one per line) or by clicking on streams in the flowsheet. Click **OK** to close the dialog box and display the report.
- **All Streams:** This report displays all stream property data for the entire flowsheet.
- **Feed Streams:** This report displays stream property data only for streams issuing from a Feed icon on the flowsheet.
- **Product Streams:** This report displays stream property data only for streams terminating in a Product icon on the flowsheet.
- **Unit Streams:** This report displays all inlet and outlet stream property data for a specified UnitOp on the flowsheet. If no UnitOp icon is selected when you run the report, you'll see the Select UnitOps dialog box; type the UnitOp ID or click the UnitOp on the flowsheet and then click **OK** to display the data. If you select a UnitOp icon before running the report, the data will display without further input.

You can quickly display stream properties for a single stream at any time, simply by right-clicking the stream in the flowsheet and selecting **View Properties**.

Particle Size Distribution

For a particle size distribution report, select **Report** > **Particle Size Distribution**. In the Select Streams dialog box, choose one or more streams for which a particle size distribution exists (one per line), either by typing in stream numbers (one per line) or by clicking on streams in the flowsheet. Click **OK** to display the report.

Pseudocomponent Curves

For a text report on pseudocomponent curves (also known as distillation curves), select **Report** > **Pseudocomponent Curves**. Select one or more streams containing hydrocarbons, either by typing in stream numbers (one per line) or by clicking on streams in the flowsheet. Click **OK** to display the report.

UnitOp-based Reports

CHEMCAD can also run reports to analyze UnitOp data. To access these reports, select the appropriate item from the **Report** menu. The results will display in either WordPad or Excel, depending on how you've configured CHEMCAD to handle text reports.

UnitOp Groups

For the UnitOps report, you can create custom UnitOp groups within a simulation. Much like their stream-based counterparts, UnitOp groups can save you time and effort when requesting reports; in addition, you can use these groups when running your simulation, to isolate and run only selected UnitOps for diagnostic or other reasons.

Note: Because of this other functionality of UnitOp groups, the order in which you list UnitOp IDs when setting up these groups is important.

The quickest way to set up any group is to use the CHEMCAD Explorer. Follow these steps to create a UnitOp group:

1. In the CHEMCAD Explorer pane, under Groups, right-click the **UnitOps** item and select **New**.
2. In the New Group dialog box, replace the default name (such as **Group 1**) with a descriptive name for your UnitOp group and then click **OK**.

Figure 8-05: Naming the new UnitOp group

3. In the Edit UnitOp Sequence Group dialog box, select the UnitOps for this group, either by typing in the UnitOp IDs (one per line) or by clicking on

UnitOp icons in the flowsheet. Add UnitOps in the order they run in the simulation. Click **OK** to close the dialog box.

As soon as you finish creating the group, its name appears under UnitOps in the CHEMCAD Explorer. From here, you can right-click the group name and select any of the following:

- **View/Edit:** Open the Edit UnitOp Sequence Group dialog box, where you can add or delete Unit Ops or reorder the existing list.
- **Rename:** Open the Rename Group dialog box, where you can type a new name for the group.
- **Copy:** Open the Copy Group dialog box, where you can type a new group name to make an exact copy of the UnitOp group. After you click **OK**, you can then edit the new copy of the group to fit your needs.
- **Delete:** Remove this UnitOp group from the simulation. If you're sure about deleting the group, click **Yes** in the dialog box that appears.
- **Run:** Run the simulation only for those UnitOps included in this group.
- **View:** Display a summary report of the UnitOps included in this group.
- **Specifications:** Bring up the UnitOp specification dialog boxes for each item in the UnitOp group, starting with the first UnitOp listed.

Note: The commands to add, edit, and remove UnitOp groups are also offered on the **Report** menu under **UnitOps**.

Select UnitOps

To run a report that covers just the Unit Ops you specify, select **Report** > **UnitOps** > **Select UnitOps**. In the Select UnitOps dialog box, specify the UnitOps you want to include in the report, either by typing in the UnitOp ID s(one per line) or by clicking on UnitOps in the flowsheet. Click **OK** to close the dialog box and display the report.

If you select a UnitOp icon before running the report, the data will display without further input.

Spec Sheet

This command exports detailed information about a UnitOp into a preformatted Excel worksheet. This report is useful for tasks such as soliciting a manufacturing quote for a piece of equipment.

- To create a spec sheet for all UnitOps on the flowsheet, select **Report** > **Spec Sheet** > **All Units**.
- To create a spec sheet only for specific UnitOps, select **Report** > **Spec Sheet** > **Select Unit**. Choose the UnitOps you want to include in the Select UnitOps dialog box, either by typing in the UnitOp IDs (one per line) or by clicking on

UnitOp icons in the flowsheet. Click OK to close the dialog box and display the spec sheet.

- For a single UnitOp spec sheet, you can select the UnitOp icon before running the report; Excel will open and the data will display without further input.

Note: For spec sheets that include multiple UnitOps, CHEMCAD creates a separate worksheet for each UnitOp's data within the Excel file that CHEMCAD creates.

Distillation

To run a distillation report, select **Report** > **Distillation** and then select one of the following:

- **Tower Profiles:** Generates a report detailing temperature, pressure, and flow rate for a distillation column
- **Tray Compositions:** Creates a report that shows the vapor flow rate, liquid flow rate, and K-value of each component on each stage of a distillation column
- **Tray Properties:** Reports on currently selected stream properties for each stage of a distillation column
- **Tower Mass Transfer:** For an SCDS distillation column that uses a mass transfer model, provides mass transfer coefficients, height of transfer units, and estimated height of theoretical plates (HETP)
- **Dynamic Column History:** Provides data from a single dynamic run of a column (described in detail in Chapter 7, *Building and Using a Dynamic Simulation*)
- **Column Diagnosis:** For columns that have not successfully converged, provides recommendations for changing column settings to achieve convergence

Flowsheet-based Reports

In addition to reports that focus on particular UnitOps and streams, CHEMCAD offers text reports that provide information about the simulation as a whole. To access any of these reports, select the appropriate item from the **Report** menu.

Topology

This report provides a listing of all UnitOps in the flowsheet, as well as all stream origins and destinations.

Thermodynamics

This report lists all components used in the simulation and provides vital information about the thermodynamics methods used.

Mass and Energy Balances

In addition to mass and energy balances, this report gives the order in which UnitOps are calculated, calculation modes used, and information about recycle loops, cut streams, and convergence.

Dynamics Reports

The **Report** menu provides access to the **Batch Results** and **Dynamics** commands, which provide reports about non-steady-stream processes.

Batch Results

This report summarizes the results of a batch distillation column simulation at the end of each operating step.

Dynamics

You can access three different reports by selecting **Report** > **Dynamics**: Dynamic Column History, Dynamic Stream History, and Dynamic UnitOp History. These reports are described in detail in Chapter 7, *Building and Using a Dynamic Simulation*.

Consolidated Report

You can run any combination of the text-based reports described above as a single operation, by selecting **Report** > **Consolidated Report**. This brings up the Consolidated Report menu.

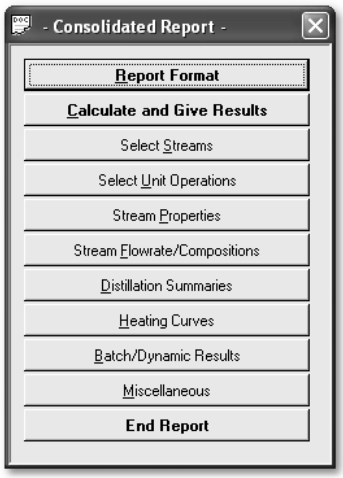


Figure 8-06: The Consolidated Report menu

From this menu, you can specify streams, UnitOps, and stream properties to include; choose flow, composition, and distillation options; and select settings for heat curves and batch and dynamic options.

To optimize your consolidated simulation report, begin at **Select Streams** and click each button in turn, customizing each dialog box with your own settings and clicking **OK** to apply your changes. When you have worked your way down the menu and set all of the options to suit your reporting needs, click **Calculate and Give Results**.

Graphical Reports

In addition to text-based reports, CHEMCAD offers a wide variety of graphical plots that you can view onscreen or print for review.

Thermophysical Data Graphs

CHEMCAD offers a number of graphical reports that relate specifically to the selected components and thermodynamics options. To access any of these plots, select the appropriate item from the **Plot** menu.

TPXY

This selection generates vapor-liquid equilibrium curves between any two components, with an optional third component. You can include TPXY, TXY, activity coefficient, and fugacity coefficient curves.

Binary LLE

This selection generates liquid-liquid equilibrium curves between any two components.

Binodal Plot

This selection generates a ternary phase diagram showing the distribution of three selected components in two liquid phases, including tie lines and plait point.

Binodal/Residue Curves

This selection creates a plot that combines the curves from a binodal plot and a residue curve plot. This is useful when working with heterogeneous azeotropic distillation.

Residue Curves

This selection generates and plots a graphical display of distillation zones, azeotropes, and residue curves associated with a user-specified ternary mixture.

Flowsheet-based Graphs

To view graphical reports that reflect your overall simulation, select one of the following from the **Plot** menu:

- **Stream Properties:** Plots one selected stream property for a selected stream in the flowsheet
- **Phase Envelopes:** Plots a phase envelope for a given stream, highlighting the critical point of the mixture; can include plots at vapor fractions other than 0 (bubble point curve) and 1 (dewpoint curve)
- **Composite Curves:** Plots composite heat curves for the entire flowsheet, as well as optional heat curves for individual UnitOps

- **Pseudocomponent Curves:** Displays a plot of one or more distillation curves for a stream

UnitOp-based Plots

CHEMCAD offers several plots that display data for a single UnitOp. To access any of these plots, select **Plot** > **UnitOp Plots** and then select one of the following options.

Tower Profiles

This selection plots compositions, temperature, and flow profiles for distillation columns.

Heat Curves

This selection plots heating and cooling curves for a selected heat exchanger.

Plug Flow Reactor Profile

This selection plots the temperature or composition profiles along the axial length of a kinetic plug flow reactor.

Pipe Profile

This selection plots fluid properties for pipe UnitOps along the axial length of the pipe. This plot requires that the pipe contain multiple segments.

Controller Convergence

For controllers that have not converged, this plot enables you to diagnose the controller behavior that is preventing convergence. The plot shows how the controller error function changes with iteration.

Dynamic Plots

CHEMCAD offers a series of plots for use with dynamic operations. Select **Plot** > **Dynamic Plots** to access any of six graphical dynamics reports.

These plots are described in detail in Chapter 7, *Building and Using a Dynamic Simulation*.

User-specified File

If you have customized CHEMCAD using VBA, C++, or other programming languages, you can save plot data into a text file and use this feature to display that data as a curve.

Select **Plot** > **User Specified File** to bring up a message box that provides instructions on how to format the text file. Click **OK** to continue to an Open dialog box, where you can select the text file you want to use. When you click **Open**, the curve is plotted and displayed.

Printing CHEMCAD Reports

You can print any text report that you produce using CHEMCAD, from within the program that you have selected to view the report.

The specific printing options differ somewhat from one program to another, but you can bring up the main Print dialog box in Word, WordPad, or Excel by selecting **File** > **Print**. Each of these programs also offers a **Print** button on the toolbar for your convenience.

For graphical reports, you can print directly from CHEMCAD. With a plot displayed, select **File** > **Print**, or click the **Print** button on the toolbar. Plots are set up to print in landscape (horizontal) orientation, as this is the best fit for the horizontal plot layout.

Process Flow Diagrams

CHEMCAD provides easy-to-use tools for creating printed process flow diagrams. You can add various types of databoxes to accompany your flowsheet, and then selectively view and print groups of items, including databoxes.

Flowsheet Databoxes

CHEMCAD offers four types of databoxes:

- **Stream Box:** Lists the streams that you select in a single table, along with the stream properties that you choose to include
- **UnitOp Box:** Generates a separate databox for each selected UnitOp
- **TP Box:** Generates separate summary databoxes for selected streams
- **Excel Range Box:** References a range of cells from an Excel worksheet

Stream Boxes

To create a stream databox, start by selecting **Format** > **Add Stream Box**. From the Select Streams dialog box, follow these steps:

1. Determine which streams to include in the databox, using one of three methods:
    - Check the *All streams* box to include all streams on your flowsheet, then click **OK**.
    - Type the numbers of the streams you want to include into the boxes provided, then click **OK**.
    - Check the *Select streams from flowsheet* box, click **OK**, and then choose the streams you want to include by clicking the actual stream lines with your primary mouse button. Stream numbers that you select will appear in the Select Streams dialog box; to toggle a selected stream off, just click it

again. When you've selected all the streams you want, click **OK** to continue.

2. Any of these selection methods will bring you to the Databox Property Options dialog box. Here, you can select which stream properties you want to include on the stream databox. You can keep the default settings, or turn any check box on or off to customize your databox.

Note: The selections you make here will be the default selections the next time you create a stream databox for this simulation.

In addition to the main **General** tab, note the **Crude/Solid** tab, which you can click to select crude oil stream properties or solid stream properties. When you've selected the stream properties you want, click **OK** to continue.

3. In the Databox Settings dialog box, you can choose the font style and size for your databox text, as well as whether to include horizontal lines or horizontal section dividers in the databox. Click **OK** to place the databox on your workspace.

As with flowsheet elements, you can move, stretch, or resize a databox using your mouse.

UnitOp Boxes

The procedure for creating UnitOp databoxes is similar to that used to create stream databoxes, with the chief difference being that there is no selection of UnitOp properties.

Begin by selecting **Format** > **Add UnitOp Box**, and then either enter UnitOp IDs or check the box to select UnitOps from the flowsheet. Note that you don't have the option of automatically including all UnitOps, as you did with streams.

When you complete your selections and click **OK**, the Databox Settings dialog box appears, with the same formatting options that are available for stream databoxes. Change any settings you want here, and then click **OK** to place the requested databoxes on your workspace.

Unlike a stream databox, which displays data for multiple items in a single box, a UnitOp databox displays data only for a single UnitOp. If you selected three UnitOps in the UnitOp IDs dialog box, you'll see three separate databoxes appear when you click **OK**. If you see only one databox at first, try moving that box to another part of the screen to see if the others are hidden behind it.

TP Boxes

CHEMCAD can create databoxes, called TP boxes, which display any combination of temperature, pressure, and flow rate for all streams or selected streams on a flowsheet.

To add TP databoxes, select **Format** > **Add TP Box**. In the TP Box Settings dialog box, first select an option at the top, to determine whether to add TP boxes for all streams or only for the streams you select.

In the **Display** column, select items from the drop-down list in each field to determine which stream properties to display and in what order. Use **No selection** as appropriate if you want to display fewer than four properties.

In the **Number format** column, make a selection in each field to determine how numbers will display in the TP boxes. In the **Digits** column, type the number of digits to display after the decimal point. You can also change the font style and size for the TP box text, and choose whether to display stream IDs and engineering units.

The **Preview** box displays a dynamic sample of how the items you've selected will appear in the TP boxes. Note that the preview area does not reflect changes you make to the font size.

When you finish making your selections in the TP Box Settings dialog box, click **OK**. If you've chosen to make TP boxes for all streams, the TP boxes will appear on the flowsheet right away. If you've opted to select the streams from the flowsheet, you'll see a Select Streams dialog box; type the stream numbers (one per line) or click on the stream lines in the flowsheet to select streams, and then click **OK** to create the TP boxes.

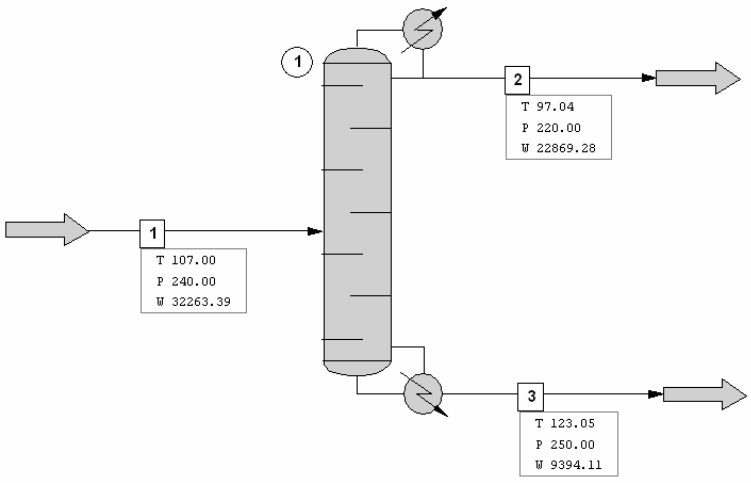


Figure 8-07: TP boxes added to a simple flowsheet

Excel Range Boxes

An Excel range box displays dynamic data from a specified cell range in a specified Excel worksheet. To create an Excel range box, follow these steps:

1. Start by selecting **Format** > **Add Excel Range**. This brings up the Excel Databox Settings dialog box.
2. Click **Browse** to navigate to the folder where the Excel workbook resides, then highlight the name of the workbook you want and click **Open**.

3. In the *Worksheet name* field, type the name of the relevant worksheet within the workbook that you've indicated.
4. In the center portion of the dialog box, specify the starting and ending column and row coordinates that you want to reference within the selected worksheet.
5. In the lower portion of the dialog box, change any formatting settings as desired and then click **OK** to create the databox.

An Excel range box is a dynamic link between CHEMCAD and the Excel worksheet. As data is updated and saved in the selected cell range, the range box can automatically update to reflect those changes. To view the most up-to-date data in your Excel range boxes at any time, select **View** > **Refresh Data Boxes**.

Using the Layers Feature for Selective Viewing and Printing

When you create a simulation in CHEMCAD, you can build your flowsheet across a huge workspace, zooming in and out as needed to work with specific areas of the flowsheet. You can also, as described above, add any number of databoxes to provide a quick visual reference for the data behind your flowsheet objects. You can add text labels, draw circles around items that you need to work on further—in short, there's practically no end to the visual clutter that could end up on your process flow diagram. But all of these elements are useful to someone, and you certainly don't want to spend your time repeatedly adding or removing visual elements before printing or sharing a PFD.

CHEMCAD's solution to visual-element overload is a feature called Layers. A *layer* is a group of objects in a simulation file—any combination of databoxes, drawn shapes, text labels, streams, and UnitOps—that you can view or hide with a single click. You define exactly which objects belong to a layer, and then toggle each layer either on (visible) or off (hidden) using the CHEMCAD Explorer.

Note: Turning off a layer does nothing beyond hiding the associated objects from view. Having a layer hidden—even if that layer includes streams and UnitOps—does not in any way affect the way the simulation runs or any stream or UnitOp properties.

Scenarios for Using Layers

The following are examples of situations in which you can use layers to enhance your process flow diagrams:

- Several different departments need to review your process flow diagram, but each department wants to see different data highlighted in databoxes. You can create one set of TP boxes listing only flow rates, for example, and then assign them all to a layer; then hide that layer and create a new set of TP boxes listing temperature and pressure only. Assign these databoxes to their own layer, hide it, and continue with stream boxes, UnitOp boxes, or

whatever other items you need. Create as many different layers as you like, and each time you go to print the diagram, view only the layers that you want to print.

- You need to e-mail a simulation to different recipients who want to view different databoxes. Create sets of databoxes assigned to multiple layers, and then view just the layers that you want your first recipient to see upon opening the file. Save and close the simulation before attaching it to an e-mail message. Open the simulation again for the next recipient, select the layers you want that person to see, save the file, and attach it to another e-mail message.
- You have a very large flowsheet that encompasses a number of discrete processes. You can create separate layers for various portions of the overall flowsheet, and view only the portions you're working with at a given time. You can also hide unneeded portions of the flowsheet for printing.
- If you are troubleshooting a process, or for whatever reason need to "mark up" a process flow diagram, you can draw shapes such as ellipses or rectangles around certain UnitOps or groups of UnitOps, using text or bright colors to draw extra attention. Then assign all of these mark-up items to a single layer so that you can choose to view either the marked-up version or the "clean" version of the flowsheet at any time.

Creating a New layer

By default, all objects are assigned to a master layer, which is always visible. Before you can assign objects to another layer, you must first create a new layer to use. The most convenient way to create a layer is within the CHEMCAD Explorer pane.

In the CHEMCAD Explorer, find the top-level item called **Layers**, right-click it, and select **New**.

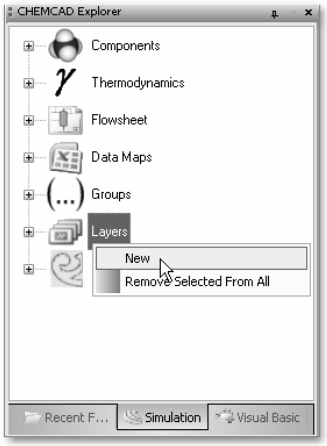


Figure 8-08: Creating a new layer

In the New Layer dialog box, replace the default layer name with a descriptive name of your own and then click **OK**.

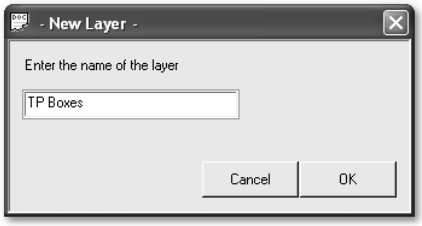


Figure 8-09: Naming the new layer

The new layer now appears under the **Layers** item in CHEMCAD Explorer. If necessary, click the plus sign next to **Layers** to view the layer name. You can add as many layers as you like and view the complete list here.

When a layer is first created, it is visible by default. A layer's status as visible or hidden is indicated in CHEMCAD Explorer by the icon that displays next to its name. A visible layer shows a green check mark, while a hidden layer is gray in color.

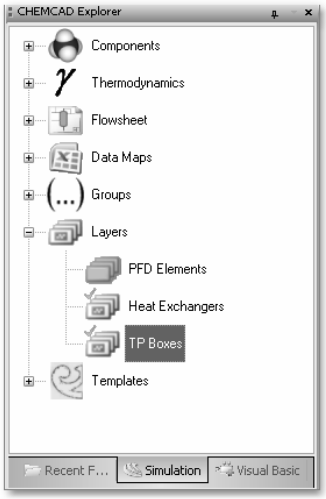


Figure 8-10: Visible and hidden layers as they appear in CHEMCAD Explorer

Assigning Objects to a Layer

Now that you have layers, you can assign items to them. Start by clicking an object to highlight it; this might be anything from a stream ID label to a UnitOp to a TP box. Whatever type of object it is, when you highlight it you'll see the four black boxes that define its outer edges. With the object selected, right-click the name of the desired layer in the CHEMCAD Explorer and choose **Add Selected**.

To save time, you can add multiple objects to a layer at once. Just hold down the **[SHIFT]** key as you click each object in turn, then right-click the layer name and choose **Add Selected**.

Note: If you like, you can assign one or more objects to a layer at the same time you create the layer. To do this, simply click the desired object (use the **[SHIFT]**-click method for multiple objects), then right-click **Layers**, select **New**, and assign the layer a name. The selected objects are automatically assigned to the new layer.

Hiding and Viewing Layers

As soon as you've added at least one object to a layer, you can test the layer by hiding it and watching what happens. To hide a layer, simply click the green check-marked icon next to that layer's name; the icon should change to gray and all items assigned to the layer should disappear from view.

At any time, you can hide or view each layer in your simulation independently. The icons next to the layer names in the CHEMCAD Explorer provide a constant reminder of which layers, if any, are currently hidden from view.

Each time you open a simulation file, CHEMCAD displays or hides its layers according to the way they were set the last time you saved the simulation.

Note: It is possible for an object to be assigned to more than one layer. If an object is assigned to two or more layers, however, it will be displayed unless *all* of its associated layers are hidden.

Removing an Object from a Layer

If you no longer want a specific object or group of objects to be assigned to a given layer, you can remove the assignment as easily as you created it.

First ensure that the layer in question is visible. Then select all the objects that you want to remove from the layer, right-click the layer name in CHEMCAD Explorer, and choose **Remove Selected**. Now when you hide the layer, the object or objects you removed should remain in view.

Deleting an Entire Layer

If for any reason you want to remove a layer from your list, simply right-click the layer's name in CHEMCAD Explorer and select **Delete**. The layer disappears from the list, and if the layer was hidden when you deleted it, the items assigned to it now reappear.

Printing a Process Flow Diagram

When you use the **Print** command on the main CHEMCAD screen, the result is a verbatim reproduction of your visible workspace.

If you're zoomed close in to one portion of your flowsheet when you print, you'll get a close-up printout that does not include the rest of the flowsheet. If you've hidden all of your databoxes to keep them out of your way while you fix a problem, those databoxes will not appear on the printout. If the Palette pane is covering up the product streams coming from one of your UnitOps, those product streams won't be on the printout either.

For this reason, the first thing you should do when you're ready to print a process flow diagram is to decide what needs to be included on the printout. If you need the entire flowsheet to appear on the printed diagram, select **View** > **Zoom Options** > **Zoom to Fit**, or zoom manually if you prefer. You may want to hide or

unpin one or more panes as well, to give yourself more workspace while you prepare to print.

Next, consider whether your process flow diagram should display a job box, UnitOp or stream databoxes, text notes, or other items in addition to the flowsheet itself. If you have already created the needed items, make sure that they are currently visible and placed where you want them.

When all of the items you want to print are visible, check once more to ensure that everything falls within the CHEMCAD workspace. Then select **File** > **Print**, or click the **Print** button on the toolbar. This brings up the Print Setup dialog box, where you can select printing options or simply click **OK** to print the process flow diagram.

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Chapter 9

Customizing CHEMCAD

As you become more familiar with the way that CHEMCAD works and the various options and tools that are available, you may find yourself wishing that you could make your own additions—either for specialized items or for those you use frequently. You can in fact customize CHEMCAD in several ways that save you time by streamlining and simplifying your workflow. These include:

- Creating stream and UnitOp templates
- Adding custom components to CHEMCAD's component database
- Making your own symbols and adding them to the UnitOps palette
- Building custom UnitOps
- Creating custom dialog boxes for UnitOp settings
- Defining custom thermophysical rules

This chapter discusses all of these types of customization, starting with the simplest procedures and then moving on to more complex customizations that require some programming experience.

Flowsheet Templates

One of the most effective ways to save time when creating CHEMCAD simulations is to make use of stream and UnitOp templates. A *template* is simply a set of characteristics, which you assign a name and save for later use. When you set up stream or UnitOp specifications that you know you'll need to recreate in the future, you can create a template of that stream or UnitOp. You can then duplicate that item within the same simulation—or in any other simulation—with just a few mouse clicks.

Creating a Template

To create a stream template, first create the stream you want to clone and give it all of the characteristics you want to include in the template.

Then find this stream on the CHEMCAD Explorer's **Simulation** tab. Expand the **Flowsheet** item, then expand the **Stream** item, and finally double-click the applicable stream ID. This brings up an item called **Save**. Double-click the word **Save** to bring up the Enter Template Name dialog box, then type a name for your new stream template and click **OK**. The new stream name is now listed beneath the **Save** item.

To create a UnitOp template, select the appropriate UnitOp ID in CHEMCAD Explorer, and then follow the same procedure used to create a stream template.

Viewing a Template's Properties

To see what specifications an existing template includes, look it up in the CHEMCAD Explorer. Expand the **Templates** item, then expand the **UnitOps** item, and finally expand the name of the relevant UnitOp type. For example, if you're looking up a template that you created for a type of pump that you frequently use, expand the **Pump** item in the CHEMCAD Explorer.

When you find your template, simply click the template name to open its specifications dialog box.

Applying a Template

To apply a stream template, first expand the CHEMCAD Explorer item for the stream in question, either by clicking the plus sign to its left or by double-clicking the stream name.

When the stream item is expanded, you'll see the **Save** item below it, followed by the names of all the stream templates that you have created. Double-click the name of the template you want to use, then click **OK** to confirm that you want to apply this stream template.

Renaming or Deleting a Template

To rename a template, simply find it under **Templates** in CHEMCAD Explorer, right-click the template name, and select **Rename**. Type the new name and click **OK**. This changes the template name throughout CHEMCAD Explorer.

The procedure for deleting a template is similar to renaming a template. Again, find the template you want under **Templates**, right-click its name, and select **Delete**. Click **OK** to confirm that you want to delete this template. The template name disappears from CHEMCAD Explorer, but streams or UnitOps that were specified using the template are not affected in any way.

Note: Any stream or UnitOp template that you create is available for use with all other simulations on the same installation of CHEMCAD, until and unless you delete the template.

Creating Custom Components

The CHEMCAD component database places detailed information about thousands of chemicals at your fingertips. If for any reason you find that you need to use a chemical component that does not match any item currently in the CHEMCAD database, you can create your own component for use with your simulations.

You can create a single component, define a range of pseudocomponents, or import a component's physical properties from an external source. These procedures have similar aims, but differ significantly from one another.

Adding a Single Component

Creating a pure component in the CHEMCAD component database is a two-part task. You must first create the component and then regress data into the component.

Creating the Component

To create a new custom component, you can use any of five different estimation methods:

- **Create a hydrocarbon pseudocomponent.** This is treated like a pure component in that certain aspects of how it behaves or reacts are known.
- **Use the Joback/Lyderson method.** With this method you indicate basic characteristics, and select molecular groups (known as Joback groups, called Group Assignments in CHEMCAD) from a list, to indicate how many of each molecular group are present in the component.
- **Use the UNIFAC method.** This method is identical to Joback/Lyderson, except that the group list is more specialized toward organic components.
- **Create a combustion solid.** This method is used to simulate solid components for which an elemental analysis and heating value are known, e.g., coal.
- **Create an electrolyte component.** This method creates a component that you can subsequently use in an electrolyte simulation.

The procedure for creating a pure component is as follows:

1. Select **Thermophysical** > **Component Database** > **Create New Component**. This brings up the New Component dialog box.

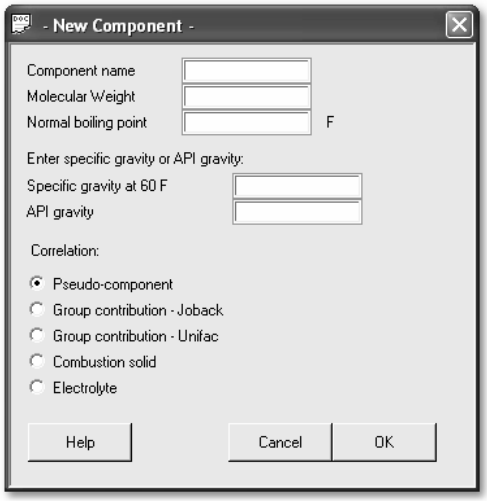

Figure 9-01: The New Component dialog box

2. Give the new component a descriptive name; it is strongly recommended that you make this name unique. All other characteristics here are optional, except for normal boiling point, which is required for the pseudocomponent method.
3. Select a **Correlation** option to indicate which of the above methods you will use, and click **OK** to continue.
4. In the resulting dialog box, select the appropriate options for your new component and specify as many characteristics as you like, as accurately as possible. Click **OK** to continue.
5. In the Select Destination Database dialog box, you will see no databases listed if this is your first time to add a component. If this is the case, click **New** to bring up the Manage Component Databases dialog box.
6. Normally, you'll need to click **Add New**, which brings up the Save As dialog box. Navigate to the location you want for your custom component database, give the database a name, and click **Save**. If you want to add a database that someone else has created (generally in a network location), you can click **Use Existing**, which brings up an Open dialog box; navigate to that database's location, highlight the database, and click **Open**.
7. The Manage Component Databases dialog box now lists the database that you created or selected. Click **OK** to continue.
8. In the Select Destination Database dialog box, the new database you have just named is now listed; highlight it and click **OK**.
9. The View/Edit Component Data menu now appears. Click any item on the menu to access a dialog box with options for defining your new component. After defining as many characteristics as possible, click **Exit** to close the menu.

The new component is now available to add to your current simulation and all future simulations. To return at any time to make changes to a user-defined component, do one of the following:

- Select **Thermophysical** > **Component Database** > **View/Edit Component** to bring up the Select Single Component dialog box, which lists all available components. Highlight the component you want in the list and click **OK** to bring up the View/Edit Component Data menu.
- Click **Component List** on the toolbar to bring up the list of components in the current simulation. Double-click the component you want in the list to bring up the View/Edit Component Data menu.

Regressing Data into the Component

Data regression is the process of fitting experimental data points to a polynomial equation form, so that the individual error of each data point is minimized.

Data regression is only relevant to temperature-dependent properties such as heat capacity, density, and vapor pressure. CHEMCAD uses these polynomial equation fits to calculate the properties of a component at any given temperature.

To regress data into a component that you have created, follow these steps:

1. Select **Thermophysical** > **Component Database** > **Component Property Regression**. This brings up the Regress Component Properties menu.

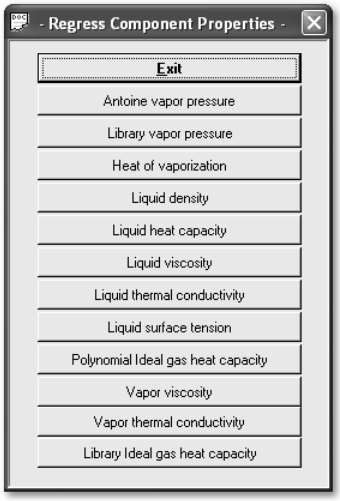

Figure 9-02: The Regress Component Properties menu

2. Click the menu item that corresponds to the type of regression data you want to enter.
3. In the Select Single Component dialog box, select the user-added component that you want to regress and click **OK**.
4. In the resulting dialog box, enter the required parameters (listed in green text) and any other parameters as appropriate, then click **OK**.

5. In the resulting dialog box, enter your experimental data points in the cells provided. You can enter a value in the **Weight_factor** column to weight the regression toward one or more data points. Click **OK** to continue.

Note: You can paste a contiguous range of cells from an Excel worksheet into the cells in this dialog box.

6. The regression data is displayed in a tabular format for review. When you are ready to view the regression curve, close the WordPad or Excel window.
7. The regression results now display in graphical format. Review the plot and decide whether the regression adequately represents your experimental data. In the Apply Component Changes dialog box, either choose an option and click **Save** or abandon your regression changes by clicking **Don't Save**.
8. Repeat this procedure as needed to regress other properties for your component, and then click **Exit** to close the Regress Component Properties menu.

Pseudocomponent Range

Using a *pseudocomponent curve*—another term for the distillation curve portion of an assay—you can cut a hydrocarbon stream into pseudocomponents, or fractions. A pseudocomponent represents a group of components that boil within a narrow temperature range. Pseudocomponent ranges are used in CHEMCAD to model hydrocarbons.

When you define a pseudocomponent range for a stream, CHEMCAD creates entries in the component database for each hydrocarbon cut, and assigns these components' compositions to the stream.

Note: Before you define a pseudocomponent range, make sure that you have specified in your component list, as appropriate, water and any light ends that exist in the assay.

1. Select **Thermophysical** > **Pseudocomponent Curves**.
2. In the Dist Curve Characterization dialog box, enter stream number(s) and click **OK**.
3. In the Hydrocarbon Correlation dialog box, select the appropriate correlations for your curve, or use the default selections and click **OK**.
4. This brings up the Curve Temperature Cut Ranges dialog box. For each cut range that you want to define, provide a beginning and ending temperature, and enter the number of points that you want to define as discrete pseudocomponents within that range. Click **OK** to continue.

5. In the Bulk Properties dialog box, specify a distillation curve type and enter a total flow rate and bulk gravity for the stream. You can make other entries here as needed, but only these three items are required. Click **OK** to continue.
6. In the resulting dialog box, enter the distillation curve from your assay, specifying the volume percentage and boiling temperature for at least five data points. Click **OK** to continue.
7. The next dialog box is optional. Enter a gravity curve from your assay, specifying the volume percentage and gravity for at least five data points. Click **OK** to continue.
8. The next dialog box is also optional. If you have light ends and water defined in your assay, enter volume percentage data here for all relevant components. Click **OK** to continue.
9. This brings up the Edit Distillation Curves menu, shown in Figure 9-03.

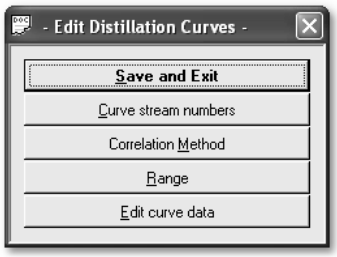

Figure 9-03: The Edit Distillation Curves menu

10. Click **Save and Exit**. This brings up a tabular listing of pseudocomponent properties. You can review and print these results if you like, or simply close the document displaying them to return to the CHEMCAD workspace.
11. To see the list of pseudocomponents that you have created, edit the properties for the stream you selected. The pseudocomponents will be listed after pure components, with names that begin with **NBP**.

Importing a Neutral File

You can also add a component to the database by importing its physical properties from an external data source. This procedure is known as *neutral file import*.

For detailed information about importing and using a neutral file, see the CHEMCAD Help system.

Creating a Custom Symbol

You can create a custom symbol in CHEMCAD, for use with either a built-in UnitOp or a user-defined UnitOp. The tool used to create symbols is called the CHEMCAD Symbol Editor.

You can launch the Symbol Editor in either of two ways:

- Within CHEMCAD, select **Edit** > **Edit UnitOp Symbols**.
- From Windows, select **Start** > **All Programs** > **Chemstations** > **Utilities** > **Symbol Editor**.

Once the editor is open, you'll see a gridded workspace and a small, free-floating tool palette.

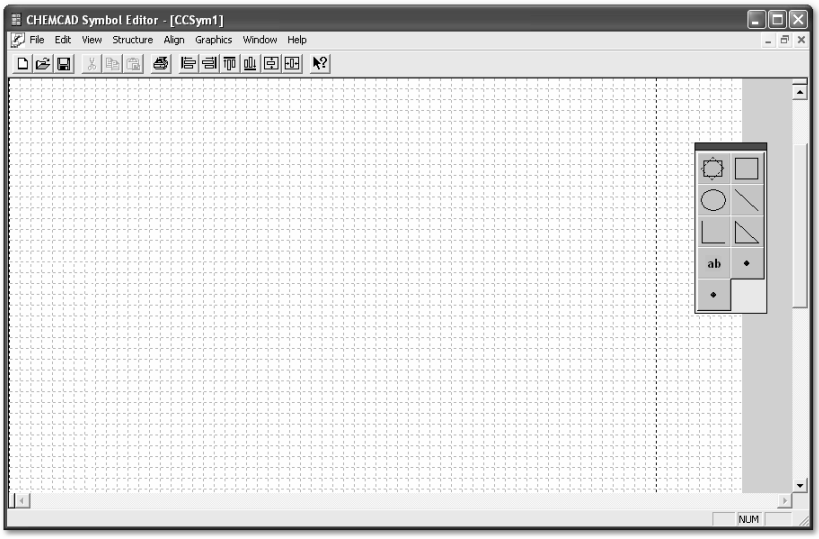

Figure 9-04: The Symbol Editor's workspace and palette

You can build a symbol from the ground up, but the best way to learn to use this tool is to edit an existing CHEMCAD UnitOp symbol. To do that, follow these steps:

1. Select **File** > **Open** from the Symbol Editor menu. In the Open dialog box, select a file from Symbols directory and click **Open**. The selected symbol opens in the Symbol Editor workspace, as shown in Figure 9-05.

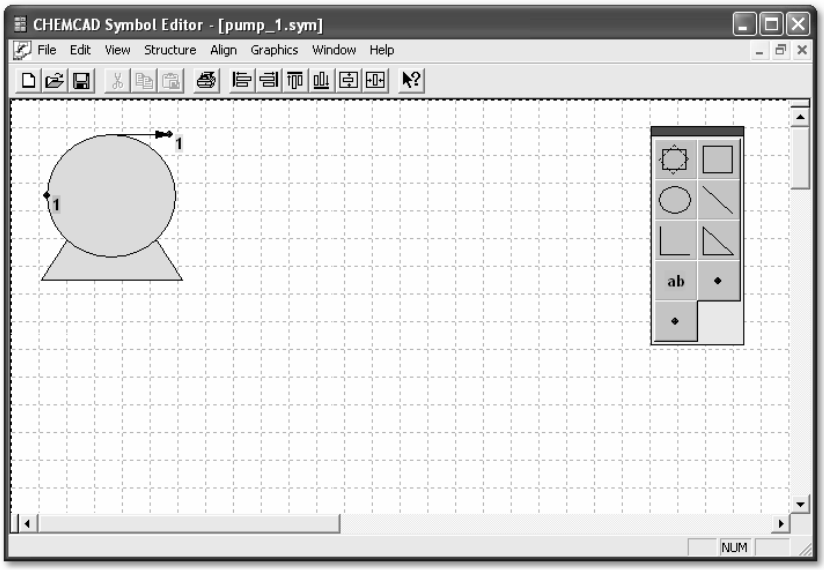

Figure 9-05: The pump_1.sym file open in the Symbol Editor workspace

2. Select **File** > **Save As** and save the file in a different directory, using a distinctive name to avoid confusion with the original symbol.
3. Use the tools available in Symbol Editor to change the symbol as needed:
   - To remove or alter any existing part of the symbol, select **Structure** > **Ungroup** to break the symbol into its individual components.
   - To add graphical components to the symbol, use the drawing tools on the tool palette, such as **Rectangle** and **Ellipse**.
   - To add a text label to the symbol, use the **Text** tool.
   - To add an inlet or outlet, click the appropriate item on the tool palette and then click to place the inlet or outlet on the symbol.
   - To back out of a change that you've made, select **Edit** > **Undo** or press **[CTRL-Z]**.
4. When you're ready to save the symbol, make sure that you have deleted any unwanted items on the workspace. Select **Edit** > **Select All** or press **[CTRL-A]**, and then select **Structure** > **Group**.
5. Select **File** > **Save** to save the changes to your new symbol.

To create a totally new symbol, simply start from a blank workspace, name the file, and use the various drawing tools to create the desired combination of shapes and text. Add inlets and outlets as needed, then group the symbol's components and save the file.

Once you've created your new symbol, you need to associate it with a UnitOp type and then add it into the appropriate UnitOp subpalette.

1. Within the Symbol Editor program, select **File** > **Edit UnitOp Type**. The Select Unit Operation Type dialog box appears.

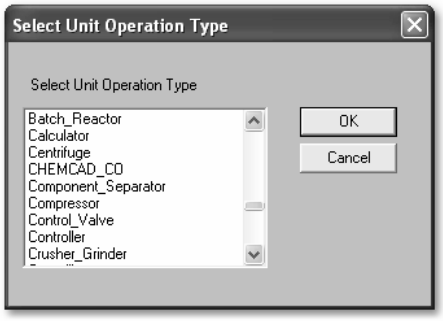

Figure 9-06: The Select Unit Operation Type dialog box

2. Select the appropriate UnitOp type and click **OK**.
3. To assign the new symbol to a UnitOp palette, select **File** > **Add to CHEMCAD Palette**.
4. Close and restart CHEMCAD to see your new symbol appear on the specified subpalette.

Customized Costing Calculations

CHEMCAD includes some very basic costing routines to help determine the capital cost of equipment. Using a simplified form of C known as the Parser language, you may modify these routines to better suit your needs.

Costing calculations are defined by a programming language called Parser, the syntax for which is documented in the *CHEMCAD Calculator/Parser Module* guide, available on the Chemstations web site.

Creating Custom UnitOps

If you need a UnitOp that falls outside the range of options offered on the All UnitOps palette, you can create a custom UnitOp. The goal of creating a custom UnitOp is to have a unit where you can enter your own equations to calculate heat and mass balances. Over the years, CHEMCAD users have created custom UnitOps for purposes as diverse as membrane separation units, fuel cells, specialized solids handling units, and crystallizers for the separation of xylenes.

Four items on the All UnitOps palette are dedicated to user-defined UnitOps. You can create a custom UnitOp using any of the following four ways:

- **Excel UnitOp:** Created through a combination of the COM interface and the Data Map interface
- **Calculator:** Created using an inline C program
- **User-added module:** Created using Visual Studio or another C++ compiler
- **VBA UnitOp:** Created through the VBA Editor, which is part of CHEMCAD

The basic procedures for creating custom Excel UnitOps are covered in Chapter 10, *Data Interfaces*. Calculator UnitOps are defined by a programming language

called Parser, the syntax for which is documented in the *CHEMCAD Calculator/Parser Module* guide, available on the Chemstations web site.

C++ user-added modules are developed using Microsoft's Visual C++ development tool, the same tools that were used in the creation of CHEMCAD's own UnitOps. The procedures for creating C++ user-added modules for use with CHEMCAD are detailed in the *User-added Modules Guide*, which is also available on the Chemstations web site.

VBA UnitOps are defined by VBA subroutines, and are described later in this chapter.

The method you choose is an important first step toward creating a UnitOp, but the choice is almost entirely up to you. Calculator UnitOps can be quick and easy to set up, but they can't do everything the other methods can. The Excel/Visual Basic approach is very powerful and uses the familiar Visual Basic language for development. A drawback to this method is that calculation can sometimes be slow due to the use of Microsoft Excel to do the calculations. The most powerful and fastest calculating method is the C++ user-added module method, but if you are new to C++, it may be challenging to use. VBA UnitOps are as powerful as those created using C++, and are much easier to build.

Whichever method you use to program the calculations of your UnitOp, you will likely need to create a dialog box to provide a user interface. A dialog box enables users to send information into your UnitOp, for example the number of stages for a distillation UnitOp. No matter what method you use to program your UnitOp, you will use the Dialog Editor program to create the user interface.

Creating a Custom UnitOp Dialog Box

CHEMCAD uses dialog boxes to set variables for all types of UnitOps. Using the Dialog Editor program, you can create a custom dialog box for use with any type of user-added units.

You can also edit an existing UnitOp's specification dialog box—for example to add text notes, to translate from English to another language, or to limit the UnitOp's functionality—although this is not commonly done.

The Dialog Editor program enables you to create and modify dialog boxes, which are controlled by files with the .MY extension. These files, along with .MAP files and .LAB files, define dialog boxes for use in CHEMCAD.

To use the Dialog Editor program, you'll need a good understanding of Windows, along with a basic knowledge of Visual Programming concepts such as objects and properties. You should also have a firm understanding of simulation in CHEMCAD before venturing into Dialog Editor.

The Dialog Editor program is separate from CHEMCAD. To launch it, select **Start** > **All Programs** > **Chemstations** > **Utilities** > **Dialog Editor**.

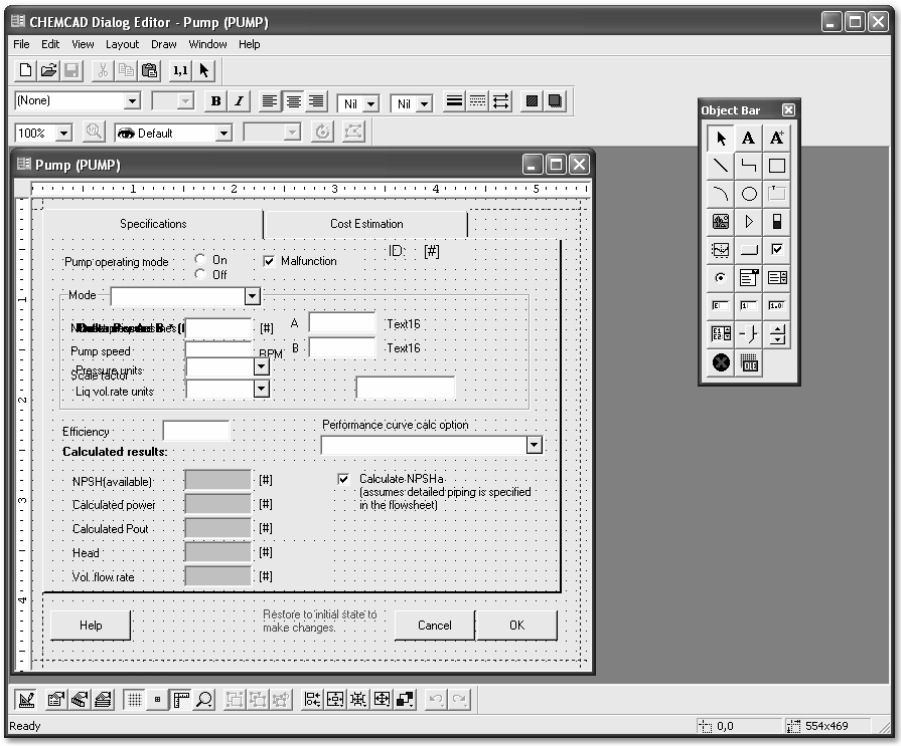

Figure 9-07: The Dialog Editor window showing an open dialog

A detailed description of how to use the Dialog Editor is available on the Chemstations web site under **Support** > **Manuals**, as well as on the CHEMCAD installation CD-ROM.

Customizing Thermodynamics

Occasionally, you may find that none of the thermodynamic models built into CHEMCAD serve your needs for a particular simulation. If this should happen, you can take one of two approaches to handling thermodynamics for the simulation: either create your own K-value or enthalpy model or create your own mixing rule.

Creating a Custom K-value or Enthalpy Model

The K-value for any component is a ratio that reflects the amount of that component present in vapor and liquid phases under given conditions. CHEMCAD uses K-values to calculate vapor-liquid equilibrium in streams and in UnitOps.

An enthalpy model calculates the heat content of a system under given conditions. Enthalpy models are used to calculate the heat balance in CHEMCAD simulations.

If you have a K-value or enthalpy method that you'd like to use, you can write C++ code to introduce your model into the CHEMCAD system. To build a custom K-value or enthalpy model using C++, navigate to the following directory to find and open the **usradd.dsw** workspace:

C:\Program Files\Chemstations\CHEMCAD\User Added Modules\usradd

This workspace includes examples of UnitOps, K- values, enthalpy models, and mixing rules.

A detailed description of how to create custom K-values and enthalpy models is available on the Chemstations web site under **Support** > **Manuals**, as well as on the CHEMCAD installation CD-ROM.

When you've successfully added a custom K-value method, you can select it on the K-value Models tab of the Thermodynamic Settings dialog box, by using the Global K-value Option setting called **ADDK**.

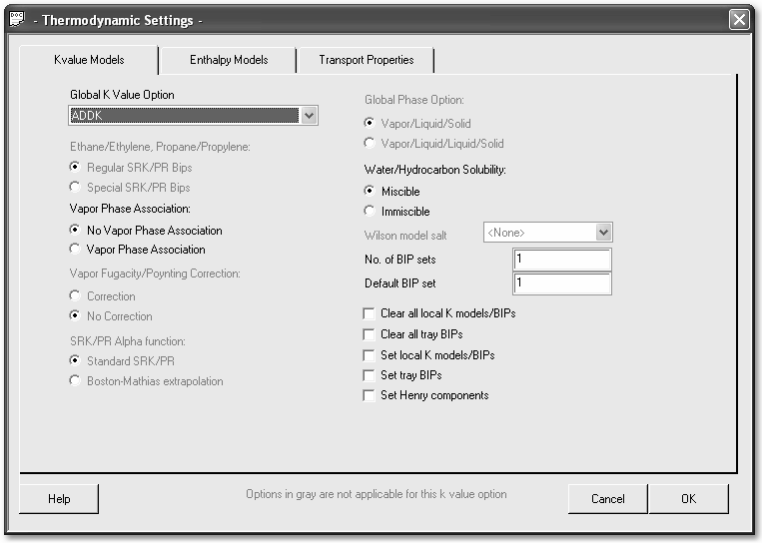

Figure 9-08: Selecting the ADDK K-value option

After adding a custom enthalpy model, you can select it on the Enthalpy Models tab of the Thermodynamic Settings dialog box, by using the Global Enthalpy Option setting called **ADDH**.

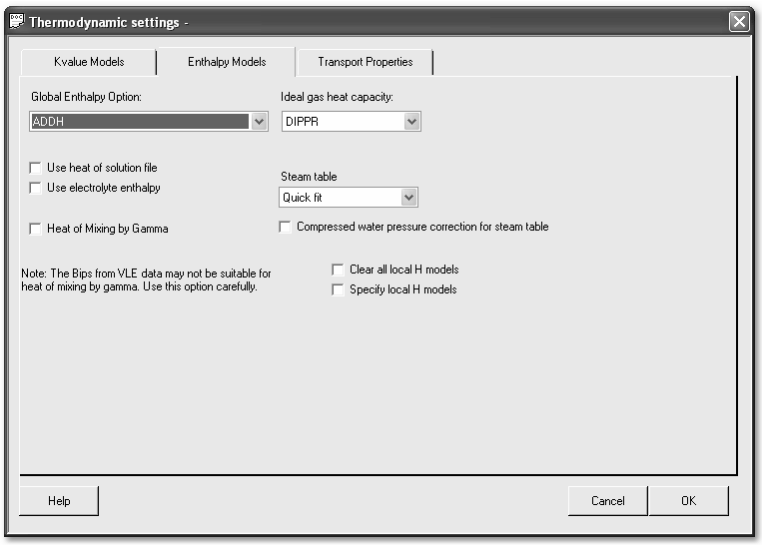

Figure 9-09: Selecting the ADDH enthalpy model

Creating a Custom Mixing Rule

A mixing rule determines how CHEMCAD calculates the properties of a mixer, based on the properties of its pure components. You can create custom mixing rules for any of the selections listed on the Transport Properties tab, either using VBA as described in the following section or using C++.

To build custom mixing rules using C++, navigate to the following directory to find and open the **usradd.dsw** workspace:

C:\Program Files\Chemstations\CHEMCAD\User Added Modules\usradd

This workspace includes examples of UnitOps, K- values, enthalpy models, and various mixing rules.

A detailed description of how to create mixing rules using C++ is available on the Chemstations web site under **Support** > **Manuals**, as well as on the CHEMCAD installation CD-ROM.

Visual Basic Applications (VBA)

You can customize CHEMCAD using Visual Basic Applications, or VBA. The CHEMCAD Explorer's Visual Basic tab provides access to the following types of customizable items:

- Reactions
- Properties
- UnitOps

If you have written code in VBA that you would like to make available in CHEMCAD, you can insert that code into one of the templates that CHEMCAD provides, or use any of these templates as a starting point and launch a VBA editor from within CHEMCAD.

Defining a Reaction, Mixing Rule, or UnitOp

To define a custom reaction, mixing rule, or UnitOp using VBA, follow these steps:

1. Click the **Visual Basic** tab in CHEMCAD Explorer and expand the relevant item: **Reactions**, **Properties**, or **UnitOps**.
2. Double-click the relevant template item to open the VBA editor.
3. Copy the existing subroutine and paste the code below the example in the code window. Rename the new subroutine copy.
4. Edit the new subroutine as needed to achieve the result that you want.
5. Return to CHEMCAD by either of two methods:
   - Use **[ALT-TAB]** or the Windows taskbar, leaving the VBA editor window open.

- Click the **View CHEMCAD** button at the far left end of the VBA editor's toolbar to close the editor window.

Note: You can also use the **[ALT–F11]** key combination to toggle between CHEMCAD and the VBA editor.

6. Save the current CHEMCAD simulation, then expand the relevant CHEMCAD Explorer item again to see your newly defined item in the list.

Using a VBA-defined Reaction

Once you have defined a new reaction, you can use it for a kinetic or batch reactor:

1. Select the **Batch Reactor** or **Kinetic Reactor** tool and place a reactor icon on the flowsheet. Add and specify streams for this UnitOp as appropriate.
2. Double-click the icon to define reactor specifications. Make the following selection to use your VBA-defined reaction.
   - **Batch reactor:** After specifying the reactor's initial charge, you'll see the Batch Reactor General Information dialog box. On the **General** tab, select the kinetic rate expression option called **Define each reaction**.
   - **Kinetic reactor:** On the **General Specifications** tab of the Kinetic Reactor dialog box, select the kinetic rate expression option called **Define each reaction**.
3. For each reaction that you define, you'll enter data into a Kinetic Data dialog box. Choose the Kinetic Rate Expression option called **User – VBA**. This brings up a drop-down list to the right of the Kinetic Rate Expression field, where you can choose a user-defined reaction. Select the appropriate option for each reaction that you define for this UnitOp, and then click **OK** to continue to the next reaction.

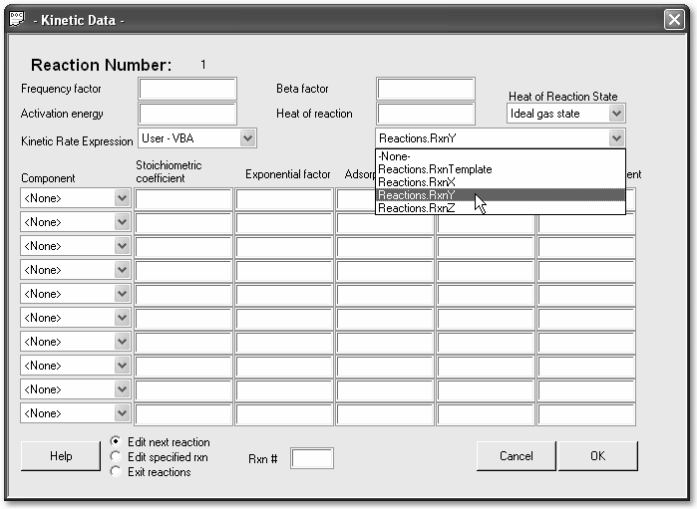

Figure 9-10: Selecting a VBA-defined reaction in the Kinetic Data dialog box

4. When you have defined the last reaction, click OK to return to the main CHEMCAD window.

Using a VBA-defined Mixing Rule

Once you have defined a new mixing rule, you can include it in your CHEMCAD simulations:

1. Select **Thermophysical** > **Thermodynamic Settings**.
2. In the Thermodynamic Settings dialog box, drop down the list of options for the mixing rule that you used as a template for your new rule. Select your rule from the list.
3. Click **OK** to return to the main CHEMCAD window.

Using a VBA-defined UnitOp

Once you have defined a new VBA UnitOp, you can include it in your CHEMCAD simulations:

1. Select the **Visual Basic UnitOp** tool and place an icon on the flowsheet. Add streams into and out of the UnitOp as you normally would.
2. Double-click the icon to define the UnitOp's specifications.
3. In the Visual Basic UnitOp dialog box, drop down the **Function** list to see the available VBA UnitOps. Select the one you want to use and click **OK**.

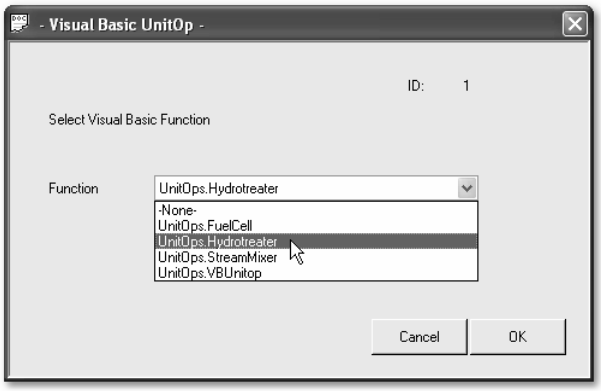

Figure 9-11: Selecting a VBA UnitOp

Chapter 10

Data Interfaces

CHEMCAD enables you to exchange data with other programs through a variety of methods. This saves time, effort, and the potential for keystroke error and data omissions. In some cases, these data interfaces can enable CHEMCAD to link directly into your plant information systems to run simulations without human intervention.

The data interfaces that CHEMCAD uses are as follows:

- The Excel Data Map interface, which can link any value in a CHEMCAD simulation to any cell in an Excel worksheet, or vice versa (note that running CHEMCAD simulations from Excel requires a COM interface, described below)
- The Visual Basic Application interface, which enables you to build custom reactions, mixing rules, and UnitOps
- The OPC interface, which permits any OPC Client application to access values in a CHEMCAD simulation
- COM interfaces, which allow any COM-enabled program (such as MATLAB) to access and control a CHEMCAD simulation

Excel Data Mapping

The Excel Data Mapping feature allows you to link, retrieve, and insert data from an Excel spreadsheet into a CHEMCAD simulation. It also lets you insert data from a CHEMCAD simulation into an Excel spreadsheet with just a few clicks. The integration of CHEMCAD and Excel is a powerful and easy-to-use tool that saves you time and work.

With Excel Data Mapping, you can quickly and easily get the most of CHEMCAD/Excel integration, even if you have no experience with Visual Basic or Excel programming. In fact, you can use and benefit from this feature even with very little knowledge of the Excel program.

To use Excel Data Mapping, you must first create one or more Data Maps, and then set up rules for the execution of each Data Map in use.

Creating an Excel Data Map

The tool used to create and edit Data Maps in CHEMCAD is the Excel Data Map Editor. This tool displays within the CHEMCAD workspace, and resembles an Excel spreadsheet. It has all you need to link stream and UnitOp parameters to one or more Excel spreadsheets. On each Excel Data Map, you can link up to 500 parameters in a single spreadsheet, and you can have up to ten Data Maps per simulation.

To link your simulation to an Excel spreadsheet, first create the target Excel workbook, making a note of the file's name, its location, and the name of the specific worksheet to which you want to link. Then follow these steps to create a new data map:

1. On the CHEMCAD Explorer, expand the **Data Maps** item and then click **New Data Map**. A spreadsheet will open within the CHEMCAD workspace.

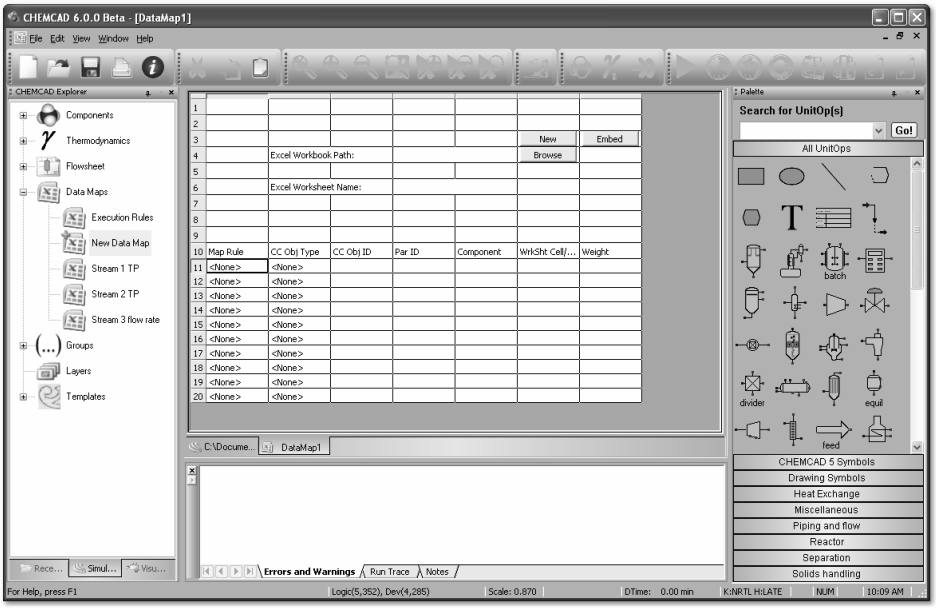

Figure 10-01: The Excel Data Map Editor

2. Click the **Browse** button and locate the target workbook. Select the workbook file and click **Open**.
3. In the cell next to **Excel Worksheet Name**, type the name of the worksheet to which you want to link your simulation.

Note: If you need to verify the name of the worksheet, you can click the **Open** button to launch Excel and view the workbook.

4. Click the cell below **Map Rule** to highlight that cell. Click again to see a drop-down list of mapping options:
   - **To Worksheet Only** enables you to send data from streams or UnitOps in CHEMCAD to the selected worksheet.
   - **To CC Only** enables you to send data from any cell on the worksheet to the selected stream or UnitOp parameter in your simulation.
   - **For data reconciliation** enables you to manipulate the data using CHEMCAD's Data Reconciliation feature.

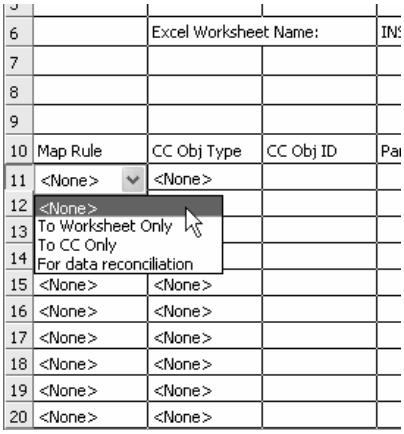

Figure 10-02: Selecting a Map Rule option in the Excel Data Map Editor

5. Click the cell below CC Obj Type to highlight that cell. Click again to see a drop-down list of mapping options:
   - **Stream** enables you to link an Excel cell or cell range to a stream on the flowsheet.
   - **UnitOp** enables you to link an Excel cell or cell range to a UnitOp on the flowsheet.
   - **Misc** enables you to change dynamic flowsheet settings.
6. Click the cell below CC Obj ID. Type the ID number of the stream or UnitOp to which you want to link.
7. Click the cell below **Par ID** to highlight that cell. Click again to see a drop-down list of parameters for the selected UnitOp or stream. Scroll down and select an option from the list.

Note: When you are importing cell data into CHEMCAD, the list of parameter options is limited, as many values in a CHEMCAD simulation are calculated based on other values.

8. If you chose a parameter that is related to a specific component (e.g., *Comp Mole fraction*, or any item marked with an arrow), you will need to specify the component. Click the cell below **Component** to highlight that cell, and click again to see a drop-down list of available components. Select a component from the list.

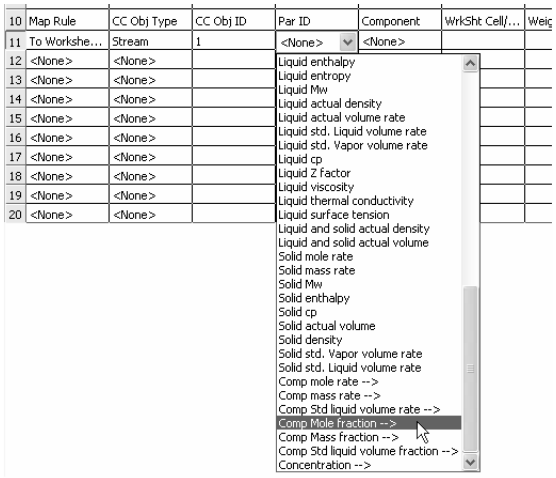

Figure 10-03: Component-specific parameters marked with arrows on the Par ID list

9. Click the cell below **WrkSht Cell/Range**. Type the cell address or cell range to which you want to link. Cell addresses should be formatted with the column letter and row number, e.g., **A1** or **D17**. Cell ranges should be formatted as two such addresses (representing the range's first and last values) separated by a colon, e.g., **A1:A12** or **B5:E20**.

10. If you are performing a data reconciliation, you can use the **Weight** column to give certain items in the reconciliation more importance than others.

11. Repeat the procedure until you have specified all of the cells or cell ranges that will link to your simulation.

12. Save the Data Map by selecting **File** > **Save As**. Type a name for your Data Map and then click **OK**. The newly created Data Map now appears on the CHEMCAD Explorer under the **Data Maps** item.

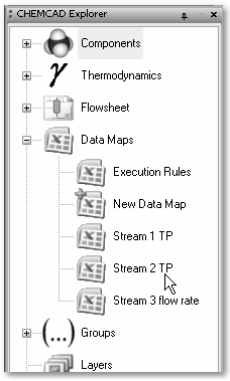

Figure 10-04: List of available Data Maps in CHEMCAD Explorer

13. To leave the Data Map open and return to your simulation, use the tabs at the bottom of the main CHEMCAD workspace. To close the Data Map, select **File** > **Close**.

Data Map Execution Rules

After configuring one or more Excel Data Maps for a simulation, you must set up execution rules to use them. You can configure up to ten Data Map files per simulation.

To set up Data Map execution rules, follow these steps:

1. On the CHEMCAD Explorer, expand the **Data Maps** item and then click **Execution Rules**. The Data Map Execution Rules dialog box appears.

Figure 10-05: The dialog box for configuring execution rules

2. Click the square button next to the first field in the *Select Data Maps* column to bring up the Select Data Map dialog box.

Figure 10-06: Selecting a Data Map from the list

3. Select the name of the Data Map for which you want to set rules, and click **OK** to return to the Data Map Execution Rules dialog box. Repeat this step for all other Data Maps whose rules you want to set up at this time.

4. In the Before Simulation Runs field next to each selected Data Map, click the drop-down list to choose an action for that Data Map to perform before calculations begin:
   - **Do Nothing** performs no action before the simulation is run. You might use this option to disable a Data Map temporarily.
   - **To Workbook** sends the requested data to Excel before running the simulation. You might use this option when you want to pull data from inlet streams or UnitOp specifications.
   - **To CHEMCAD** sends the requested data in Excel to CHEMCAD before running the simulation. You might use this option when you want to feed data to inlet streams or UnitOps with data from the Excel worksheet.
5. In the After Simulation Runs field next to each selected Data Map, click the drop-down list to choose an action for that Data Map to perform after calculations are complete:
   - **Do Nothing** performs no action after your simulation has run. You might use this option to disable a Data Map temporarily.
   - **To Workbook** sends the requested data to Excel after running the simulation. You might use this option when you want to send data from streams or calculated parameters of UnitOps to the workbook in Excel.

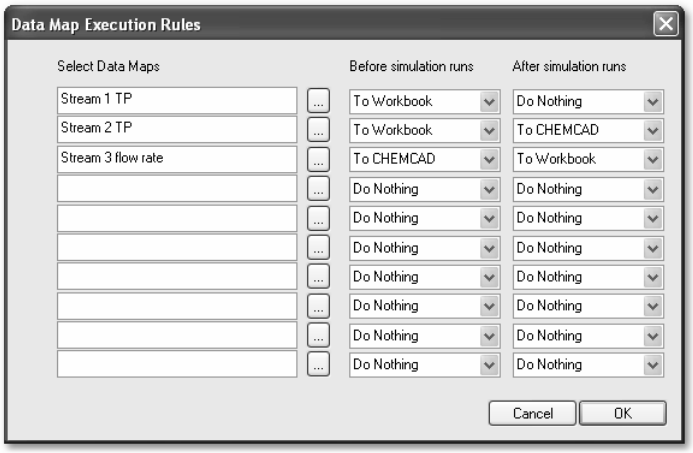

Figure 10-07: Three different Data Maps with rules set up

6. When you have configured all of the Data Maps that you want to use, click **OK** to save your rules and close the Data Map Execution Rules dialog box.

You can now run the simulation. If you open the Excel files that are linked to the simulation, you will be able to see the parameters of streams and UnitOps related to the Excel Data Map. You can also perform your own calculations in the workbook based on the data linked to CHEMCAD.

Creating Excel UnitOps

You can build an Excel spreadsheet that functions as a UnitOp within CHEMCAD. This is useful for extremely simple UnitOps such as mixers and dividers, or for simple separations.

1. Start by creating a custom dialog box for your new UnitOp, as described in Chapter 9, *Customizing CHEMCAD*.
2. Next, create an Excel spreadsheet containing your desired calculations for the new UnitOp.
3. Open a simulation, select the **Excel UnitOp** tool on the All UnitOps palette, and place a UnitOp icon on the workspace.
4. Draw the appropriate streams into and out of the Excel UnitOp.
5. Double-click the UnitOp icon to open the Excel WorkBook Unit dialog box.
6. On the File Paths tab, use the top **Browse** button to specify the location and file name of the custom dialog box that you created. Use the second **Browse** button to specify the location and file name of the Excel workbook.
7. Now you need to specify how this spreadsheet will link to CHEMCAD. Click the **Data Maps** tab to link the spreadsheet using one or more Data Maps, or click the **Excel Macros** tab to link the spreadsheet using the COM interface.
   - On the **Data Maps** tab, specify the execution rules as described earlier in this chapter.
   - On the **Excel Macros** tab, specify the names of the Excel macros that you have programmed to use the COM interface, in the order that you want them to be calculated.
8. Click **OK** to return to the main CHEMCAD window.

Specification Sheets

Using the interface with Microsoft Excel, CHEMCAD allows you to output simulation data to an Excel spreadsheet resembling a vendor specification sheet, as discussed in Chapter 8, *Output and Reports*. Customizing these spec sheets saves you time by outputting data in the format required by your company or vendor.

To customize the spec sheet for a specific UnitOp type, edit the corresponding Excel spreadsheet in the following directory:

C:\Program Files\Chemstations\CHEMCAD\Program\templates

If the UnitOp type you want is not represented by the Excel files in this directory, you can copy the generic **specsheet.xls** file and use it as a template for a new UnitOp spreadsheet.

Place the copy in the same directory, and make its file name the standard four-character abbreviation for the UnitOp type in question. For example, to create a spec

sheet template for the Flash UnitOp, you would need to name the file copy **flas.xls**. See the CHEMCAD Help information about your specific UnitOp if you need to look up this abbreviation.

Before you continue, you will need to turn off the Read-only attribute for the new spreadsheet file. The quickest way to do this is to right-click the file within the Windows Explorer, select **Properties**, and then clear the **Read-only** check box in the Properties dialog box.

Once the copy is renamed and the Read-only attribute is turned off, you can open the spreadsheet and edit it as needed.

Using CHEMCAD as an OPC Server

CHEMCAD is capable of setting up an OPC server which allows direct data transfer between any CHEMCAD simulation and any OPC client application.

OPC stands for *OLE for Process Control*. OPC provides a standard method for different devices and applications to share data. Using OPC, you can share data between CHEMCAD simulations and SCADA systems, data historians, distributed control systems (DCS), and human-machine interfaces (HMIs).

In fact, the acronym *OPC* is now considered by many to mean *Openness, Productivity, Connectivity*, because this technology forms the basis for sharing and manipulating plant data.

OPC-enabled systems are classified as either *OPC servers* or *OPC clients*. OPC servers are either applications or devices that provide data. OPC clients are interfaces that use and manipulate this data. OPC clients can connect to multiple OPC servers at any time and read and write data to all of them.

OPC Applications

OPC can be applied as follows:

- **Inferential sensors:** Sometimes called *soft sensors*, inferential sensors use one or more measured variables to estimate another variable. Using CHEMCAD simulations and data from your plant's DCS, you can embed simulations to provide data such as concentrations, heat duty, and fouling factor, which would not normally be available.
- **Operator training:** You can couple an operator HMI to a dynamic simulation to create a training simulator that can help train operators in a safe and effective way.

OPC Compliance

Chemstations is a Member of the OPC Foundation, an organization devoted to maintaining the OPC standards. CHEMCAD has been certified for, and interop tested for, OPC DA standard 2.05a.

Enabling CHEMCAD as an OPC Server

To enable OPC within CHEMCAD, select **Tools** > **Options** > **Misc. Settings**, then check the **Enable OPC Server** box and click **OK**. When you do this, CHEMCAD registers an OPC server named **CHEMCAD.SimulationServer.1** on your machine.

Once you load a simulation, all of that simulation's stream properties and UnitOp settings and variables are automatically published as tags to the OPC server's namespace.

Every value tag has a units tag associated with it, which shows the engineering units used to report the value. To change the engineering units, select **Format** > **Engineering Units** within a CHEMCAD simulation.

When the OPC server feature is enabled, CHEMCAD automatically registers itself as an OPC server. If you want to unregister CHEMCAD and remove it from the list of OPC servers, you can select **Start** > **Run** and type the following command:

```
{program directory}\CC6.Exe -unregister
```

For example, if your program directory were **C:\Program Files\Chemstations\CHEMCAD\Program** (the default directory), you would type the following:

```
C:\Program Files\Chemstations\CHEMCAD\Program\CC6.exe -
unregister
```

Reading and Writing Values to CHEMCAD Using OPC

You can use OPC to have values read from or written to a simulation, and to run the simulation. Both steady-state and dynamic simulations can be run in this way.

Values are updated to the OPC server whenever CHEMCAD completes a steady-state run or a dynamic time step. Values can also be read; in the case of a dynamic simulation, reading values between time steps will cause the program to extrapolate from the last converged results.

Values can be written at any time. If CHEMCAD is in the process of executing a time step or a steady-state simulation, the values are held in a buffer until the simulation is converged, at which time the values are written to CHEMCAD.

When values are written to a CHEMCAD stream, the stream is immediately reflashed, and all OPC tags for that stream are updated.

OPC Server Operations

In addition to reading and writing process data to CHEMCAD, it is useful to be able to send commands to CHEMCAD, for example to tell CHEMCAD to start or stop running a simulation.

This is done with a series of flags in the CHEMCAD group of the OPC server. To use any of these flags, write a 1 to flag. CHEMCAD will execute the desired command and return a value indicating success or failure. A return of 0 indicates

that the command has completed successfully, while a negative return indicates a problem of some kind.

The available commands are as follows:

- **Refresh Server** tells CHEMCAD to refresh all data sent to the OPC server.
- **Run Steady State** runs a steady-state simulation. When the simulation finishes, the flag will be reset either to 0 (run converged) or to a negative number indicating the number of errors that occurred during the run. To view the error message text, you must open the CHEMCAD interface directly.
- **Restore to initial state** returns a dynamic simulation to time zero. A return of 0 indicates success; a value of -1 indicates failure.
- **Run Dynamic** starts a dynamic simulation. A return of 0 indicates success; a value of -1 indicates failure.
- **Run Dynamic One Step** runs a single time step of a dynamic simulation. A return of 0 indicates success; a value of -1 indicates failure.
- **Set Initial State** sets the current process conditions as the time-zero conditions, overwriting the previous time-zero conditions. A return of 0 indicates success; a value of -1 indicates failure.
- **Stop Simulation** stops a dynamic simulation. A return of 0 indicates success; a value of -1 indicates failure.

CHEMCAD OPC Namespace

An OPC namespace defines and organizes all the available commands and data. OPC namespaces are divided into groups, each of which contains items. Items are sometimes referred to as *tags*.

Note: Most of the data items in a simulation have engineering units associated with them. In these cases, we usually define two separate tags, one containing the data value and the other containing the units string. All units strings are read only from OPC. The units strings are governed by the settings inside the simulation.

The groups in CHEMCAD's OPC namespace are organized as follows:

- **CHEMCAD.SimulationServer:** This is the OPC server name. By convention, this name is followed by a version number, e.g., **CHEMCAD.SimulationServer.1**, to indicate the OPC Server version. This is the server name to which OPC clients will connect.
- **CHEMCAD Group:** This group contains any information that is not dependent on a stream or UnitOp, and all commands used to run CHEMCAD.

- **Streams Group:** This group contains a series of subgroups, one for each stream on the flowsheet numbered by stream ID number.
- **UnitOperations Group:** This group contains a series of subgroups, one for each unit operation on the flowsheet, numbered by UnitOp ID number.

COM Interfaces

Component Object Model (COM) is a Microsoft-standard platform that enables programs to share content such as data and calculation routines. This interface makes it possible for other programs to control a CHEMCAD simulation.

CHEMCAD acts as a COM server, so any program that can act as a COM client can be made to interface with CHEMCAD in this way. If you aren't certain whether your application can act as a COM client, check with the software vendor.

Note: Using the COM interface to CHEMCAD is a complicated procedure that requires some experience in programming. If your organization lacks in-house expertise in programming, consider bringing in a third-party resource to assist you with the procedure.

The following section is a brief walk-through of a simple COM interface between Excel and CHEMCAD.

Connecting Excel and CHEMCAD: A Simple COM Interface

While you can export or import data values using Excel Data Map, more complicated interactions—such as running a simulation from another program—require the extra control afforded by the COM interface.

The following is a simplified description of the procedure for connecting these two programs and enabling Excel to load a simulation, change a value, run the simulation again, read the same value, and then close the simulation.

In this procedure, you'll use Excel to do the following:

- Open CHEMCAD
- Read in values from CHEMCAD into an Excel workbook
- Change a value in the simulation
- Run the simulation
- Read the revised values back into Excel

Normally, using COM interfaces involves some programming. We have created an example called VBCLient.xls to help you overcome that hurdle; you don't need to write any code at all to use this tool. Even if you need to write your own program, the code in the macros of VBClient will come in handy as a guide.

Using the VBClient Example

Follow these steps to use the VBClient example:

1. Open Excel and load the workbook called **VBClient.xls**. This workbook has three worksheets:
   - **Command** contains buttons for controlling a CHEMCAD simulation.
   - **Streams** displays all stream data in the simulation. This sheet can be used for both input and output of stream variables to the CHEMCAD simulation.
   - **UnitOps** displays all UnitOp-related data for the simulation. This sheet can be used for both input and output of UnitOp variables to the CHEMCAD simulation.
2. On the Command sheet, you will see a series of buttons to load CHEMCAD, load a simulation, read data from the simulation, write data back to the simulation, and run the simulation. Click **Load CHEMCAD** to start an instance of CHEMCAD.

   Click **Load Simulation** to load a simulation into CHEMCAD.

   Make a change to the data shown on the Streams and UnitOps sheets.

Note: Some values are read-only. For example, VBClient does not allow you to change a stream's total flow rate directly; you must instead change the component flow rates to make a change to the total flow rate.

3. Click **Save Data** to push your changes to the CHEMCAD simulation.
4. Click **Run All** to run the simulation.
5. Note the changes to the data on the Streams and UnitOps sheets.

A Peek under the Hood

Right-click **Load CHEMCAD**, select **Assign Macro**, and then click **Edit**. The Visual Basic editor in Excel opens to display the code behind the button:

```
Sub LoadCC5()

   ' initialize global variables
   selJobName = ""
   selCaseName = ""
   selUpdateStrUopData = False
   selOK = False

   Set CC5 = Nothing

   ' load CHEMCAD
```

```
    Set CC6 = CreateObject("CHEMCAD.VBServer")

    If CC6 Is Nothing Then
       Dim msg As String
       msg = "Can not load CHEMCAD."
       MsgBox msg

    End If
End Sub
```

The most important line in that whole subroutine is:

```
Set CC6 = CreateObject("CHEMCAD.VBServer")
```

In that single line, Excel loads CHEMCAD into memory.

Loading a simulation is accomplished with this simple line:

```
retFlag = CC6.LoadJob(casePath)
```

Running a simulation can be as simple as this:

```
retFlag = CC6.SSRunAllUnits
```

The document called **COM Interface Reference.doc**, available on the Chemstations web site, provides a full reference of the commands available through COM.

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Chapter 11

CHEMCAD Tutorials

Although the simulations stored in your Examples directory are useful for many scenarios, the best way to learn to use CHEMCAD is to create and run simulations yourself. The tutorials in this chapter walk you through basic simulation building step by step, using a realistic example problem that will help prepare you for your own simulations.

The first tutorial is for a simple steady-state simulation, which is then used as the basis for the second tutorial, in which you'll learn to use the CC-THERM module to rate a heat exchanger. The third tutorial walks you through a batch distillation problem using CC-BATCH, and the final tutorial covers various scenarios for piping systems.

CC-STEADY STATE Tutorial

This tutorial creates a basic steady-state simulation for a condensate stabilizer plant. In this plant, gas enters the system with the feed conditions shown in the following diagram:

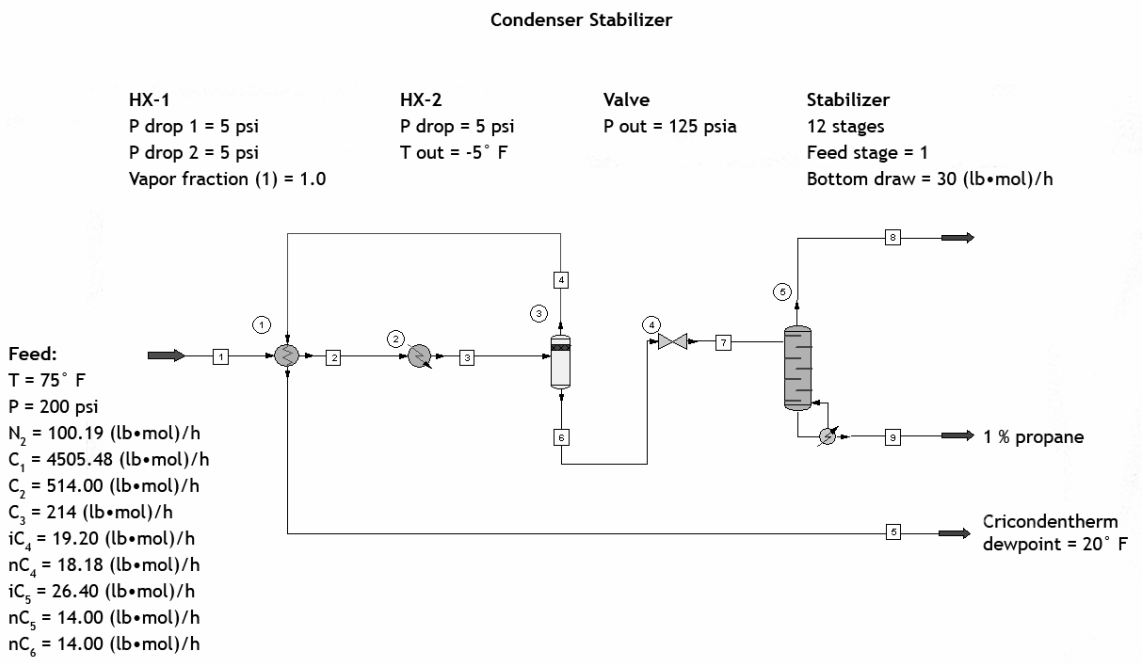


Figure 11-01: Condenser stabilizer problem diagram

Your job is to determine new operating conditions for this existing plant, along with any necessary modifications. The design requirements are as follows:

- The cricondentherm dewpoint of the product gas must be 20° F or less. A cricondentherm dewpoint is the highest temperature for two-phase coexistence of a mixture. As long as the stream temperature stays above the cricondentherm dewpoint, the stream contents will not condense.
- The stabilized condensate must have maximum propane content of 1%.

Overview

Running a flowsheet simulation in CHEMCAD is essentially a nine-step procedure:

1. Start a new simulation.
2. Select engineering units.
3. Create a flowsheet.
4. Select components.
5. Select thermodynamics options.
6. Define the feed streams.
7. Enter UnitOp parameters.

8. Run the simulation.
9. Review the results and print as needed.

The steps do not have to be performed in this order, nor do all of them have to be done for each flowsheet, but you should consider all steps for each problem.

Starting a New Simulation

Start by creating a new simulation and giving it a name.

To do this, launch CHEMCAD and then Select **File** > **Save** to open the Save As dialog box. Navigate to the directory where you want to store the simulation (try My Simulations, located under My Documents) and give your simulation a name, leaving the type as **CHEMCAD 6 (*.cc6)**. Then click **Save** to create the file and return to the main CHEMCAD window.

Note: Instead of saving all changes instantly, CHEMCAD now saves your simulation only when you use the **Save** command. This provides you with greater flexibility and gives you more control over your simulations, but it also means that you should save your work frequently. This is a sound practice for working in any software application, as it can help you avoid losing work in the event of a power problem or computer glitch.

Selecting Engineering Units

Select **Format** > **Engineering Units** to open the Engineering Unit Selection dialog box.

The **English** units option is the default and is currently highlighted. To change the engineering units system, you would click the **Alt SI**, **SI**, or **Metric** button; you could then change any of the individual units as well. For this tutorial, you will use English units, so click **Cancel** to exit this dialog box without making changes.

Drawing the Flowsheet

As described in Chapter 5, creating a flowsheet is a matter of placing UnitOp icons on the screen, connecting them with streams, and then adding various graphical objects to enhance the drawing.

Placing UnitOps

1. Start your flowsheet by adding an icon to represent the initial feed stream. In the All UnitOps palette, find the **Feed** icon, which is an arrow pointing to the right. Click the **Feed** icon, then click in the workspace where you want to place the feed stream. When the feed stream arrow appears, go ahead and turn off the **Feed** drawing tool by right-clicking any blank area of the workspace.

Note: At any time after drawing a feed stream or any UnitOp icon, you can click the icon to display the black sizing handles at each corner. With the icon selected this way, you can click the icon and drag it to a new location, or click any sizing handle and drag it outward or inward to resize the icon.

2. Now place the two heat exchangers on the flowsheet. On the All UnitOps palette, point to the **Heat Exchanger** icon until its pop-up label appears (see Figure 11-02).

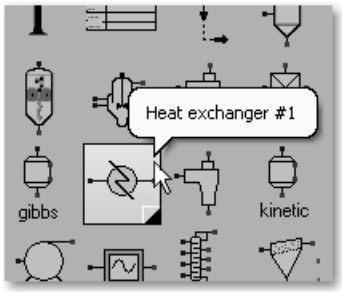


Figure 11-02: The pop-up label that identifies the UnitOp icon

3. Click the lower right corner of the **Heat Exchanger** icon, on the black triangle, to open the sub-palette. Select the two-sided heat exchanger icon as shown in Figure 11-03. The icon that you clicked in the sub-palette now appears on the main All UnitOps palette to represent the Heat Exchanger UnitOp.

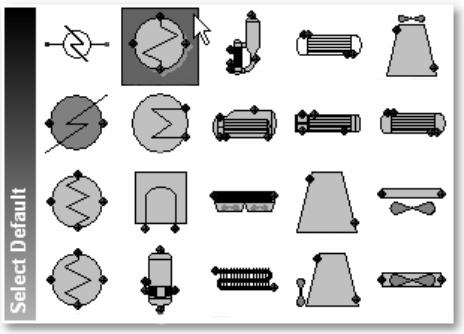


Figure 11-03: Selecting the two-sided heat exchanger icon

4. Point the mouse cursor about an inch to the right of the feed icon and click. A two-sided heat exchanger icon appears on the flowsheet where you clicked.

Note: The UnitOp ID label of **1** should appear in a circle next to the heat exchanger icon. For each subsequent UnitOp that you draw, CHEMCAD will assign an ordinal number in this way, to uniquely identify each piece of equipment on the flowsheet.

5. Return to the All UnitOps palette, and again click the **Heat Exchanger** icon's black triangle. To switch from the two-sided model to a single-sided model, you'll need to select the appropriate icon (see Figure 11-04) from the Heat Exchanger sub-palette.

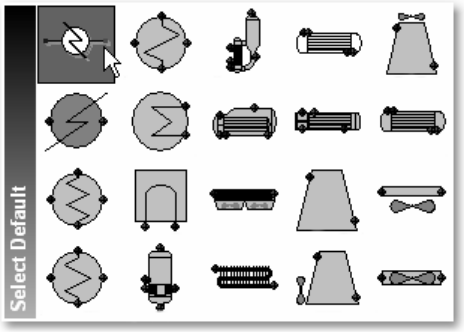


Figure 11-04: Switching to the single-sided heat exchanger icon

6. Again move the cursor to the workspace, this time about an inch to the right of the first heat exchanger, and click the mouse. A single-sided heat exchanger icon appears on the flowsheet where you clicked. Your flowsheet so far should look something like Figure 11-05.

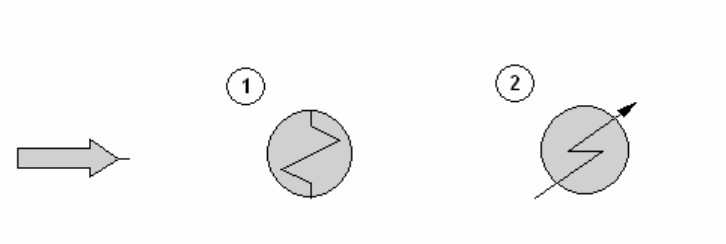


Figure 11-05: The flowsheet so far

7. Add the Flash and Valve UnitOp icons to your flowsheet, using the standard icons.

8. For the condensate stabilizer, use a distillation column. Multiple distillation UnitOps are available, but for now, assume that the module you want to use is the rigorous distillation model called *Tower*. You'll need a Tower icon with trays and a reboiler but no condenser; this is different from the default Tower UnitOp icon. Click the lower right corner of the Tower icon's box to view the sub-palette, then select the icon shown in Figure 11-06.

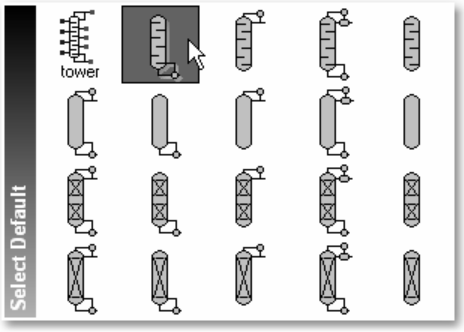


Figure 11-06: Selecting the appropriate Tower UnitOp icon

9. Now that you have selected the appropriate Tower icon, add this UnitOp to the flowsheet.

10. Place three Product icons on the flowsheet, one for each product stream. You can quickly place three identical icons, simply by clicking repeatedly in a slightly different location. When you've clicked to create the third Product icon, right-click to turn off the Product drawing tool.

Drawing Streams

Now that all of the UnitOps are in place, select the **Stream** tool and connect the various UnitOps as appropriate. Remember that each stream must start at a red outlet point on the upstream UnitOp, and end at a blue inlet point on the downstream UnitOp.

To avoid having to re-select the Stream tool each time, make sure that as soon as you click to complete one stream, you move the cursor to the next location and click to start the next stream.

Draw streams to connect the following:

- Feed stream to first heat exchanger's left-side inlet
- First heat exchanger's right-side outlet to second heat exchanger's left-side inlet
- Second heat exchanger's right-side outlet to flash inlet of your choice
- Flash top outlet to first heat exchanger's top inlet
- First heat exchanger's bottom outlet to nearest product icon
- Flash bottom outlet to valve inlet
- Valve outlet to tower inlet of your choice
- Tower top outlet to nearest product icon
- Tower bottom reboiler outlet to nearest product icon

As you draw streams, CHEMCAD assigns stream IDs, just as it assigned UnitOp IDs when you created those items. The labels for stream IDs are displayed in squares, to distinguish them from the UnitOp IDs displayed in circles.

Selecting Components

Now you need to identify the components to be used in this simulation. Start by selecting **Thermophysical** > **Select Components**. This brings up the Select Components dialog box, shown in Figure 11-07.

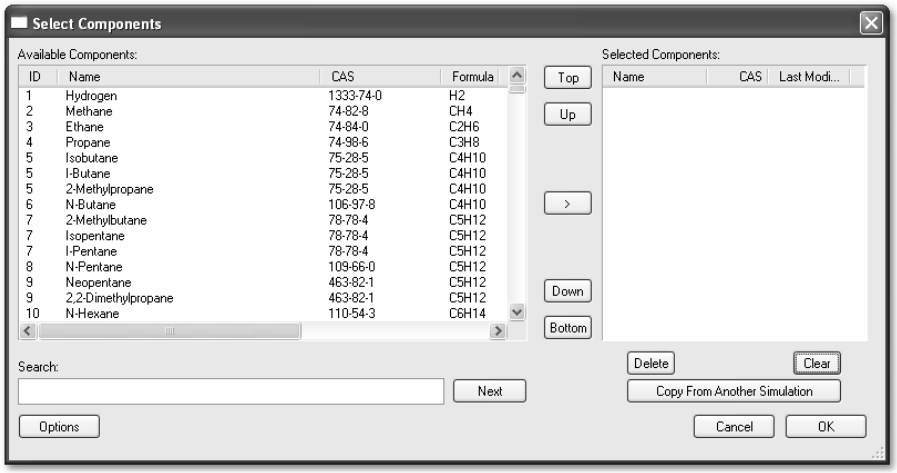


Figure 11-07: The Select Components dialog box

For this example, you'll choose components from the standard CHEMCAD database. In the Select Components dialog box, find and add each needed component, beginning with nitrogen:

1. In the Search box, start typing the word **nitrogen**.
2. As soon as you've typed **ni**, you should see *46 – Nitrogen – N2* highlighted in the *Available Components* area. Click the right arrow button to add nitrogen to your simulation.
3. Use the scroll bar in the *Available Components* area to return to the top of the component list.
4. Hold down the **[CTRL]** key on your keyboard as you click each of the following components in turn:
   - 2 Methane
   - 3 Ethane
   - 4 Propane
   - 5 I-Butane
   - 6 N-Butane
5. Click the right arrow button, located to the right of the *Available Components* area, to add all of the selected components to your simulation.
6. Now add the following components by double-clicking each one in turn:
   - 7 I-Pentane
   - 8 N-Pentane
   - 10 N-Hexane

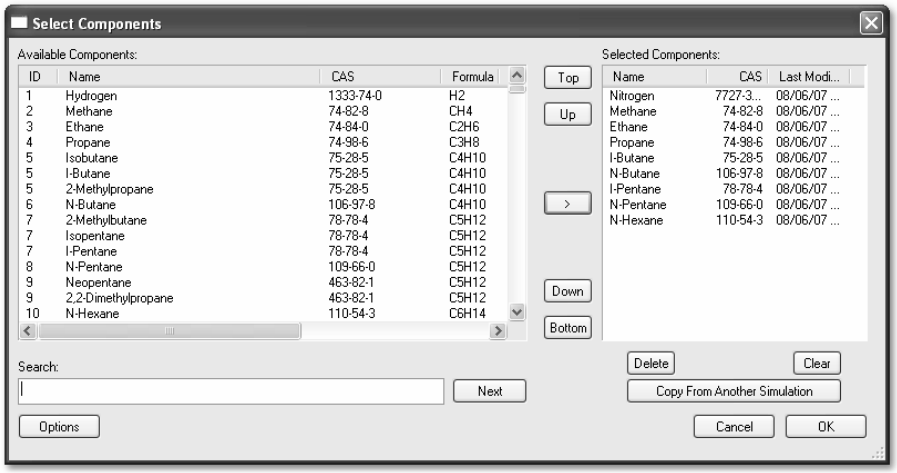


Figure 11-08: The completed Select Components dialog box

7. Save your component selections by clicking **OK**.

Selecting Thermodynamic Options

As soon as you have finished component selection, the Thermodynamics Wizard appears. This tool can suggest thermodynamics options to use with this simulation.

CHEMCAD's Thermodynamics Wizard works like this:

1. First, it looks at the component list and decides what general type of model is required, i.e., equation-of-state, activity model, etc.
2. Second, it looks at temperature and pressure ranges that you provide and decides which equation within a given category is best at the limits of those ranges.
3. If the method is an activity model, the program then looks at the BIP database to see which model has the most data sets for the current problem. It then calculates the fractional completeness of the BIP matrix. If that fraction is greater than the BIP threshold parameter, it uses the chosen activity method; if not, it uses UNIFAC.

The Thermodynamics Wizard is no replacement for engineering judgment. This tool uses an algorithm based on general rules, and is therefore fallible. The suggested model might not always be the best model for the system.

Selecting thermodynamic options basically means selecting a model or method for calculating vapor-liquid (or vapor-liquid-liquid) phase equilibrium (called the *K-value option*) and selecting a method or model for calculating the heat balance (called the *enthalpy option*). The commands for these selections are located on the Thermophysical menu.

CHEMCAD has a library of dozens of K-value models with a variety of options and about 12 enthalpy models. Making the proper selection from these libraries can sometimes be difficult. For the purposes of this tutorial, assume that you want to use

the Peng-Robinson method for both the K-value and enthalpy calculations. Follow these steps to select your thermophysical options:

1. Accept the default temperature and pressure ranges in the Thermodynamics Wizard and click **OK**.
2. Click **OK** again to accept the wizard's suggested method of SRK.
3. When the Thermodynamic Settings dialog box opens, find the Global K-Value Option selection, in the upper left corner of the K-Value Models tab. The current setting is **SRK**, but for the purposes of the tutorial, you'll need to select the Peng-Robinson model. Click the down arrow at the right end of the selection box to view a long list of K-value choices, then click **Peng-Robinson**.

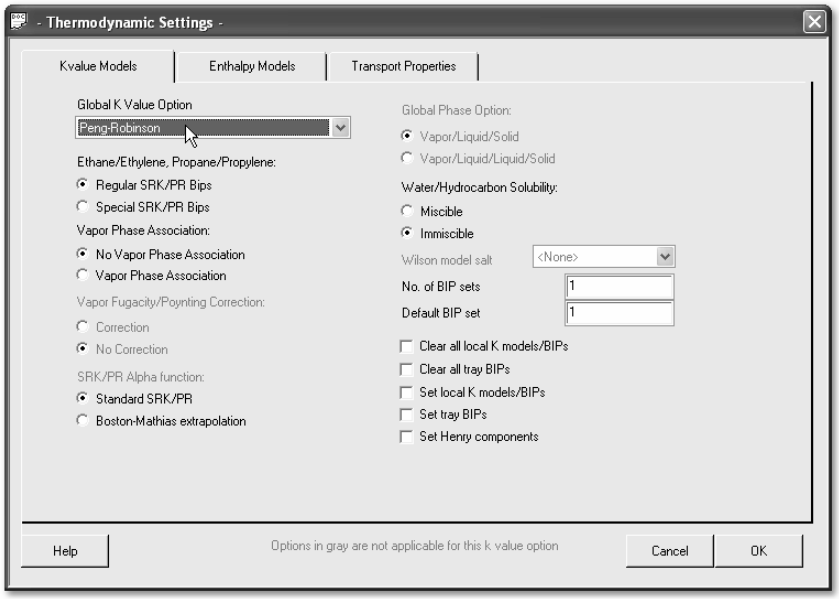


Figure 11-09: The new K-value selection in the Thermodynamic Settings dialog box

4. Now click the **Enthalpy Models** tab. The Peng-Robinson method has already been entered as the Global Enthalpy Options selection; this was done automatically because you chose Peng-Robinson as your K-value method. While you do have the option to override this choice, in this case you'll need to keep the Peng-Robinson model; leave all settings as they are and click **OK** to return to the main CHEMCAD workspace.

For the purpose of this tutorial, the thermodynamic selections are now complete.

Note: While you are not required to use the Thermodynamics Wizard, you should know how to use it, if only as a starting point for your simulations. You can revisit the wizard at any time by selecting **Thermophysical** > **Thermodynamics Wizard**.

Defining the Feed Streams

Now it's time to define your simulation's feed stream. There are several ways that you can do this, but the quickest and most efficient way to define a single stream is to double-click the stream line.

Note: Before you proceed, verify that your engineering units are set to **English** in the Engineering Unit Selection dialog box, as described earlier in this tutorial.

Double-click the line for stream 1, your feed stream, to bring up the Edit Streams dialog box.

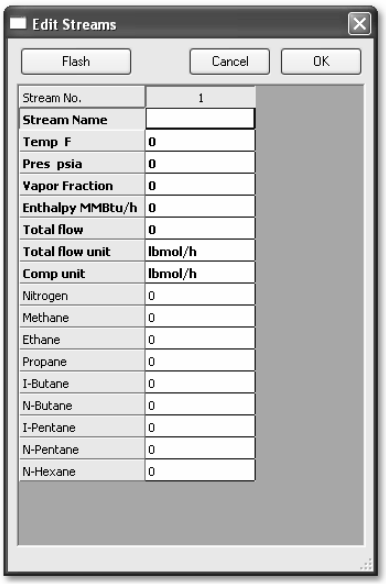


Figure 11-10: The Edit Streams dialog box

You will specify the feed stream according to the following rules:

- The **Stream Name** field can display a stream label of up to 16 alphanumeric characters. This field is optional, and you can use any label you like.
- The next four fields—**Temp F**, **Pres psia**, **Vapor Fraction**, and **Enthalpy MMBtu/h**—are the *thermodynamic properties* of the stream. According to the Gibbs Phase Rule, once a mixture's composition is given, specifying any two of these four thermodynamic properties will define the other two. As such, defining the composition, temperature, and pressure for a mixture uniquely defines its vapor fraction and enthalpy. Alternatively, defining the composition, pressure, and enthalpy will uniquely define the mixture's temperature and vapor fraction.

  Since enthalpies are calculated relative to a datum, the calculation of any given stream enthalpy is an involved process which is prone to errors. For this reason, CHEMCAD does not permit you to enter stream enthalpy as a constraint.

In addition to defining the stream's composition, you must define exactly two of the following properties: temperature, pressure, and vapor fraction. The two variables that you specify will display as red text, while the third variable and the value enthalpy will be displayed in black when you flash the stream.

An exception to this convention allows you to add heat duty with an empty stream. If you specify a total component flow rate of zero, you may specify a temperature, pressure, and enthalpy rate. A stream defined this way is treated as a heat duty, and is added to the heat balance of the unit. The temperature and pressure are arbitrary for this situation.

- The **Total flow unit** and **Comp unit** fields work together to provide a variety of ways to define stream compositions. If the selected comp unit is mole, mass, or volume fraction (either globally or locally), then the **Total flow unit** selection is available. If the selected comp unit is a flow or amount option, then the total flow rate becomes the sum of the component flow rates, and the **Total flow unit** selection is not available.
- If the **Comp unit** field selection is an amount flow unit (as opposed to a fractional unit), then the component flow rate values are automatically added as you enter them. The current sum is displayed in the **Total flow** field.
- You can click the **Flash** button at any time to perform a flash calculation using the currently specified composition and thermodynamic properties. This enables you to obtain flash calculations quickly and without leaving the dialog box.
- Fractions that do not add up to 1.0 are automatically normalized when you either click **Flash** or exit the dialog box.

With these rules and behaviors in mind, enter the data for your feed stream.

1. Begin with the stream temperature. Click the **Temp F** label, then click the empty field to its right. Type **75** and then press the down arrow key on your keyboard to continue.
2. Type **200** in the **Pres psia** field, then press the down arrow key several times until you arrive at the **Nitrogen** field.

Note: Before you continue, verify that the **Comp unit** field is set to **lbmol/h**.

3. Type **100.19** in the **Nitrogen** field, and then in similar fashion, type the following numbers in the corresponding fields:
    - Methane: **4505.48**
    - Ethane: **514**
    - Propane: **214**
    - I-Butane: **19.2**

- N-Butane: **18.18**
- I-Pentane: **26.4**
- N-Pentane: **14**
- N-Hexane: **14**

4. Click **OK** to save this stream information and return to the main CHEMCAD workspace.

Enter UnitOp Parameters

Now that you've specified your feed stream properties, it's time to specify the characteristics of your UnitOps. The following sections address each UnitOp in turn.

Note: As with streams, you can enter UnitOp parameters in various ways, but for the purposes of this tutorial, we'll use the quickest and simplest method, double-clicking each UnitOp to access its specification dialog box.

First Heat Exchanger

1. Double-click the flowsheet icon for the first heat exchanger. The Heat Exchanger dialog box will appear, as shown in Figure 11-11.

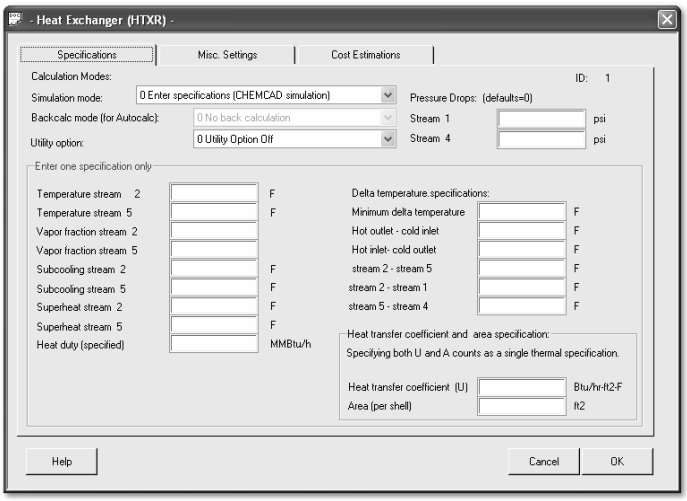


Figure 11-11: The Heat Exchanger dialog box

2. As with many types of UnitOps, the dialog box for specifying a heat exchanger consists of multiple tabbed pages. You can browse through the **Specifications**, **Misc. Settings**, and **Cost Estimations** tabs by clicking each tab in turn.

3. The pressure drop on both sides of this exchanger is 5 psi. On the Specifications tab, find the *Pressure Drops* area, and enter **5** in both the *Stream 1* and *Stream 4* fields.

4. The first stream outlet must be at its dewpoint, so you'll need to specify an outlet vapor pressure of 1. In the field next to *Vapor fraction stream 2*, enter **1**.

5. Click **OK** to save the specifications for this UnitOp and close the dialog box.

Second Heat Exchanger

1. Double-click the flowsheet icon for the second heat exchanger. The Simple Heat Exchanger dialog box will appear.
2. The outlet temperature from this heat exchanger will determine how much of the liquid is removed in the flash drum. This, in turn, will determine the cricondentherm dewpoint of the product gas. Therefore, this specification is one of the key parameters of this process. As a first attempt, use an outlet temperature of -5° F. Enter **5** in the *Pressure drop* field and **–5** in the *Temperature of stream 3* field.

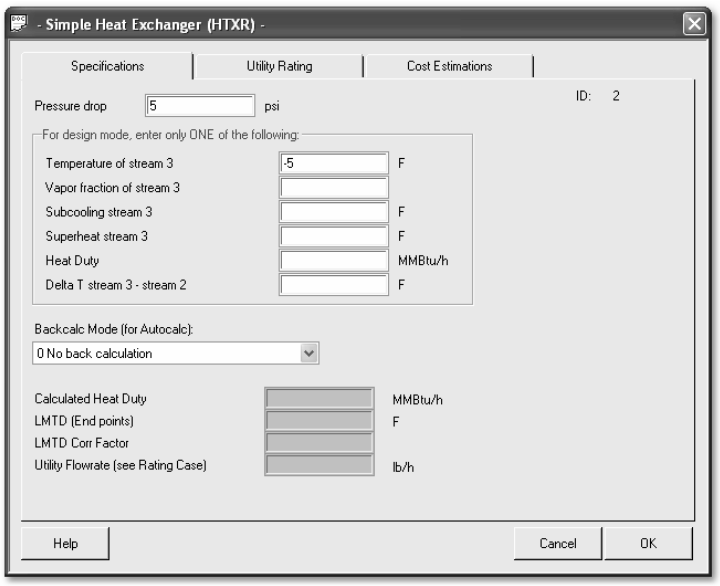


Figure 11-12: Setting up the second heat exchanger

3. Click **OK** to save the specifications for this UnitOp and close the dialog box.

Flash Drum

In this simulation, the flash drum is a vapor-liquid separator and requires no specification.

Valve

1. Double-click the valve flowsheet icon to bring up the Valve dialog box.
2. The outlet pressure for this unit is 125 psia, so enter **125** in the *Outlet pressure* field.
3. Click **OK** to save the specifications for this UnitOp and close the dialog box.

Stabilizer Tower

1. Double-click the tower icon to open the TOWR Distillation Column dialog box. Note that the settings for this UnitOp are divided into five tabs.
2. On the **General** tab, enter the following:
   - Colm press drop: **5**
   - No. of stages: **12**
   - Feed tray for stream: **1**
3. Click the **Specifications** tab to make specifications for the column. This column has no condenser or side streams, so you will only be making specifications for the reboiler. Drop down the list of options for *Select reboiler mode*, and select the mode called **4 Bottom mole flowrate**.
4. Now you need to specify the numeric value of the reboiler flow rate. In the *Specification* field immediately to the right of your reboiler mode selection, enter a value of **30**.
5. Click **OK** to save the specifications for this UnitOp and return to the main CHEMCAD workspace.

All of the data entry for the flowsheet is now complete. Before you continue, you should save your simulation. As noted earlier, it's a good idea to do this periodically as you build the simulation, but completion of your UnitOp specifications is a particularly good time to stop and save.

Run the Simulation

To run the simulation, click the **Run All** button on the toolbar.

The program first rechecks the data and lists any errors and warnings in the Messages pane. In this case, you should have no errors, although you will have warnings about estimates you have not given. You can ignore these warnings and proceed by clicking **Yes**. The calculation will then proceed.

When the run finishes, a message box appears: *Recycle calculation has converged*. To close this dialog box and clear the screen, click **OK**.

Review the Results and Print as Needed

Before running and printing reports and plots, you should review the simulation to verify whether it meets the design criteria set out for this problem.

Checking the Cricondentherm Dewpoint

If you have chosen the proper outlet temperature for the second heat exchanger, the cricondentherm dewpoint for the product gas stream (stream 5) will be 20° F or less. The cricondentherm dewpoint, you will recall, is the highest dewpoint temperature a mixture will ever see at any pressure. The simplest way to identify the highest

dewpoint temperature of the product gas is to plot all of the dewpoint temperatures of the product gas, i.e., to plot a phase envelope.

1. Start with the Plot menu, which provides access to all types of graphical reports. Select **Plot** > **Phase Envelopes**. In the Select Streams dialog box, specify stream **5**, then click **OK** to bring up the Phase Envelope dialog box.
2. No entries are required on this screen since you only need to look at the dewpoint line, but to make the plot more interesting, display the 0.25 and the 0.5 vapor fraction lines in addition to the normal phase envelope boundaries. Complete the dialog box as shown in Figure 11-13.

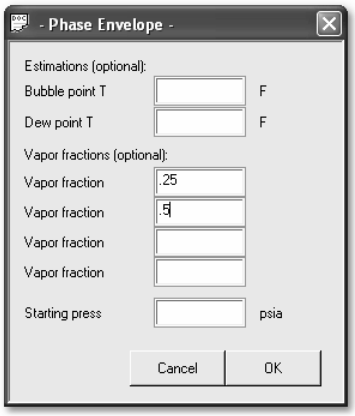


Figure 11-13: Plotting vapor fraction lines along with the cricondentherm dewpoint

3. Click **OK** to continue. CHEMCAD perform the required flash calculations to generate the specified phase envelope. Phase envelope results are produced in two formats:
   - A numerical tabulation (table) of the temperature, pressure, vapor fraction, vapor compressibility factor, and the liquid compressibility factor
   - A graphical plot of temperature and pressure for each vapor fraction line requested

   The tabular results will appear first; since you're interested in the graphical results, close the window displaying the table. The screen will now look similar to Figure 11-14. Note that the main CHEMCAD button toolbar is largely unavailable now, and the menu items have changed.

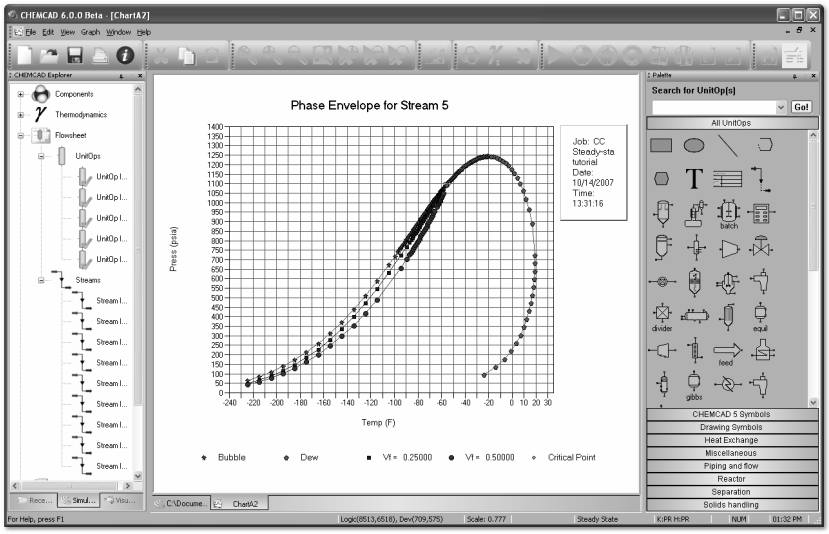


Figure 11-14: Phase envelope plot results

4. To determine whether the cricondentherm dewpoint of stream 5 is 20° F or less, zoom in on the far right portion of the dewpoint curve. To do this, click and drag with your mouse to highlight that portion of the graph—approximately 400 to 1000 psi and 0 to 30° F. When you release the mouse button, the selected area will fill the entire plot window, giving you a close-up view of specific data points.

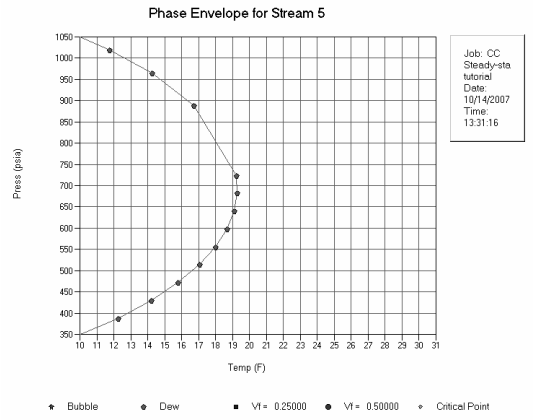


Figure 11-15: Zoomed-in plot results

5. As this view shows, the highest dewpoint of this mixture is a little less than 20° F, so the cricondentherm dewpoint is indeed within the target product gas specification. Right-click the mouse anywhere in the plot window to return to the full plot view.

6. To print the phase envelope plot, click the **Print** button and then follow any prompts from your printer.

7. You can also try the following to practice working with plots in CHEMCAD:

   - Edit the text of the plot title (in this case, *Phase Envelope for Stream 5*) or the graph axis labels by selecting **Graph** > **Edit Titles**. In the Chart Titles

dialog box, make any desired changes and then click **OK** to view the updated chart.

- Select **Graph** > **Edit** to open the Chart Explorer, which provides access to settings for color, size, layout, and various other aspects of the plot presentation.

8. Return to the main CHEMCAD window by selecting **File** > **Close**.

Checking the Bottoms Stream Purity

This problem also requires that the percent of propane in stream 9 be 1%. You can check to see if you've achieved this specification by checking the stream composition report available on the **Report** menu. First, though, you'll need to set the flow units for the stream composition.

1. Select **Report** > **Set Flow Units** to bring up the View Flow Rate Unit dialog box. Click the **Mole %** button and then click **OK** to apply this selection and close the dialog box.
2. Now select **Report** > **Stream Compositions** > **Select Streams**. In the Select Streams dialog box, enter **9** and then click **OK** to continue.
3. The resulting tabular data window shows that propane is greater than the 1% specification (see Figure 11-16). This means that the initial design is too conservative. To correct this, you can go back and re-specify the column to produce precisely 1% propane in the bottom.

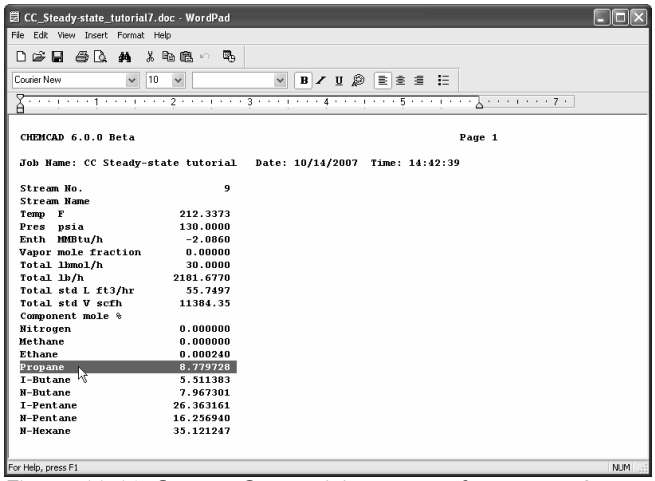


Figure 11-16: Stream Composition report for stream 9

4. Select **File** > **Exit** in the tabular data window to return to the main CHEMCAD window.

Re-running the Simulation

You can now re-run the stabilizer, specifying that you want 1% propane in the bottom.

1. Double-click the Tower UnitOp to bring up the TOWR Distillation Column dialog box for the stabilizer.
2. Click the **Specifications** tab. You need to change the reboiler mode from **4 Bottom mole flowrate** to a purity specification. Click the *Select reboilers mode* drop-down list and select **6 Bottom component mole fraction**.
3. With this change of mode, you need to specify the desired purity and the component for which it is being specified. In the *Specification* field, enter **.01**. In the *Component* drop-down list, select **4 Propane**.
4. Click **OK** to save your changes and return to the main CHEMCAD workspace.
5. You can now re-run the calculations for the condensate stabilizer. While you could accomplish this using the **Run All** command, it's more efficient to re-run only the UnitOp that you have changed. The quickest way to do this is to right-click the UnitOp icon on the flowsheet and select **Run this UnitOp**. Run the Tower UnitOp using this method.

As soon as you see the *Run finished* message in the bottom left corner of the CHEMCAD window, you can check on the propane content of the bottom stream. You've already seen how to get a detailed Stream Composition report; you can also use the Flowsheet Quickview feature to get instant stream information without even clicking the mouse.

Find the **Flowsheet Quickview** button at the far right end of the CHEMCAD toolbar. If this button is not currently activated (with a thin outline and a white button background), click the button to turn on this feature.

Figure 11-17: Turning on the Flowsheet Quickview feature

With Flowsheet Quickview turned on, point your mouse cursor at stream 9 on the flowsheet. After a moment, a pop-up information window appears, listing stream properties including composition. The value for propane should be 1 or very close to 1, as shown in Figure 11-18.

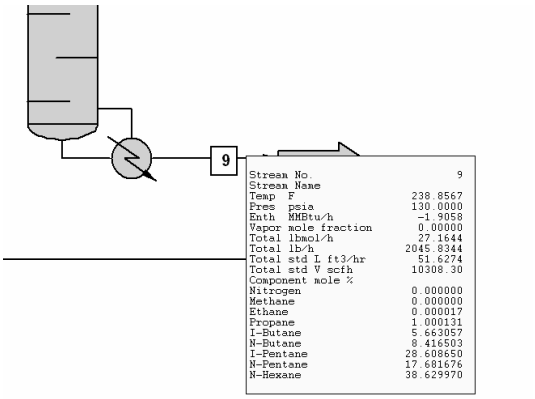


Figure 11-18: Checking the propane content of stream 9

Now that you have achieved the results that you set out to produce, save the simulation, using either **File** > **Save** or the **Save** button on the toolbar.

Producing a Text Report

The Report menu offers a broad array of text reports, as described in Chapter 8, *Output and Reports*. For the purpose of this tutorial, assume that you want to view and print out a report with the following information:

- For Streams 1, 5, 8 and 9, the stream composition in mass flow rates and mole fractions, as well as the default stream properties
- The equipment summaries for every piece of equipment in the flowsheet
- Tower tray profiles for the condensate stabilizer

Because you want a report with a broad range of information about your simulation, use the Consolidated Report option.

1. Select **Report** > **Consolidated Report** to bring up the Consolidated Report menu. From here, you can specify exactly what you want to include in your report.
2. Start by specifying which streams you want to include. Click **Select Streams** to open the Select Streams dialog box.
3. Click the **All streams** box to clear the default check mark, then type the numbers **1**, **5**, **8**, and **9** into stream ID boxes. Click **OK** to return to the Consolidated Report menu.
4. Now select which UnitOps you want to include. Click **Select Unit Operations** to open the Select UnitOps dialog box.
5. The **Print all UnitOps** option is selected by default. In this case, you do want to include all UnitOps in the report, so verify that this box is checked and then click **OK** to return to the Consolidated Report menu.
6. Click **Stream Properties** to open the Property Options dialog box. Here, you can select any combination of items on the **General** and **Crude/Solid** tabs to determine what stream properties will be included in the report. Checked

items will be included by default; to toggle any item on or off, simply click the corresponding box.

For the purpose of this tutorial, use the default settings in this dialog box. Click **Cancel** to close the dialog box and return to the Consolidated Report menu.

7. Click **Stream Flowrate/Compositions** to open the Flow/Composition Options dialog box. Click the checked box next to **Mole flow rate** to turn off this default option. Then, click the **Mass flow rate** and **Mole fractions** boxes to turn both of those options on. Click **OK** to save your settings and return to the Consolidated Report menu.
8. Finally, specify which information to print for the condensate stabilizer distillation column by clicking **Distillation Summaries**. In the Distillation Options dialog box, the information you're looking to print—**Tray profile**—is already selected. Click **OK** to return for the last time to the Consolidated Report menu.
9. To generate the report, click **Calculate and Give Results**. The report displays in a separate window, with a format suitable for printing. You can edit, save, and print the report as needed.
10. When you finish reviewing and working with the report, close the report window to return to the main CHEMCAD workspace.

Generating a Process Flow Diagram

As you know, the streams and UnitOps on a flowsheet only tell part of the story of your process. Fortunately, CHEMCAD provides many features to help you add the extra content needed to turn a plain flowsheet into a full-fledged process flow diagram (PFD) for others to review and use.

To prepare your finished simulation to be printed as a PFD, you'll add a stream databox containing the heat and material balance for the entire flowsheet. You'll place that databox underneath the flowsheet diagram and then add a title to the area above the flowsheet. Finally, you will create a new layer in this simulation and assign the PFD-specific items to that layer, so that you can hide them from view when working and display them again quickly for printing.

Follow these steps to prepare and print the PFD:

1. Start by zooming out to give yourself more workspace. If you use a mouse that is equipped with a scroll wheel between the mouse buttons, you can point at the center of your flowsheet and roll the scroll wheel down a few clicks to zoom out. If you don't have a scroll wheel, you can select **View** > **Zoom Options** > **Out**.
2. Now place the databox containing the heat and material balance for this flowsheet. Select **Format** > **Add Stream Box** to bring up the Select Streams

dialog box. Because you want to include all streams, leave the settings the way they are and click **OK** to continue.

3. In the Databox Property Options dialog box, review the default selections, indicated by checked boxes. For the purposes of this tutorial, leave the selections as they are and click **OK** to continue.
4. In the Databox Settings dialog box, you can control the font style and size of the databox text, as well as the use of dividing lines within the box. Accept the default settings here and click **OK**.
5. The stream databox appears in the upper left corner of the CHEMCAD workspace, but you want to place it below the flowsheet. The databox is already selected, so point your mouse cursor anywhere inside the box and then click and drag to reposition it. Move the databox until it is centered below the flowsheet diagram.

Note: You can also resize a databox by selecting the box and then clicking and dragging any of the sizing handles at the corners. Drag in to make the databox smaller, or out to make it larger; notice that the text adjusts in size to fit the box.

6. Now place a title on the PFD to describe the process. In the All UnitOps or Drawing Symbols palette, find and select the **Text** tool.
7. Move the cursor to a point somewhere above the flowsheet and click the primary mouse button. A vertical insertion point line begins to blink where you have clicked. Type the words **Condensate Stabilizer PFD** and then click any blank spot on the CHEMCAD workspace.
8. To make this text larger, select **Format** > **Font**. In the Font dialog box, change the **Size** setting to **18** and then click **OK**.
9. Click and drag the new heading to center it above the flowsheet diagram.
10. Finally, set up a layer for your stream databox and title so that you can display or hide these items as a single unit. At the bottom of the CHEMCAD Explorer pane, click the **Simulation** tab, then right-click the **Layers** item and select **New**.

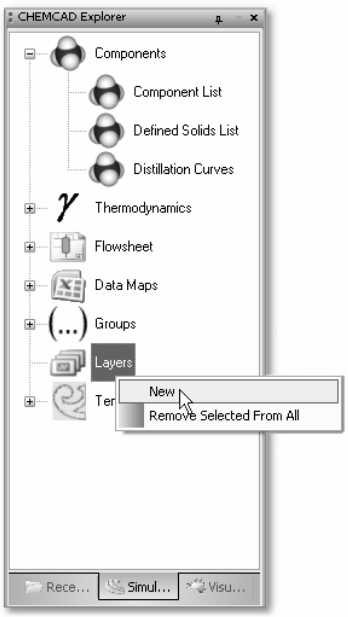


Figure 11-19: Creating a new layer using the CHEMCAD Explorer

11. In the New Layer dialog box, type a name for the new layer. For this example, name the layer **PFD Elements**, then click **OK** to create the layer.

12. Now add the two PFD elements to the layer. Click the title that you placed above the flowsheet, then hold down the **[SHIFT]** key and click inside the stream databox that you placed below the flowsheet. Both items should now be selected, with small black boxes visible in each corner.

13. In the CHEMCAD Explorer pane, double-click the **Layers** item to expand it, then right-click on your newly created **PFD Elements** layer and click **Add Selected**.

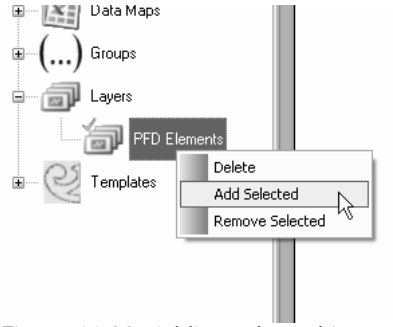


Figure 11-20: Adding selected items to your new layer

14. The title and stream databox are now part of the **PFD Elements** layer. This layer is visible, as indicated by the green check mark on its icon. Click this icon or the name **PFD Elements** to toggle the layer off, causing the title and stream databox to disappear; then click again to make them visible.

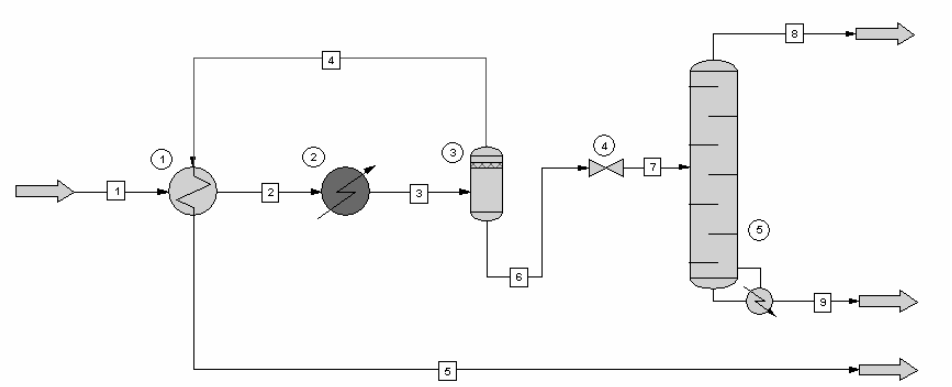
15. With the PFD elements visible, select **View** > **Zoom Options** > **Zoom to Fit**. This custom-fits the entire PFD to the available workspace for optimal printing. To print, you can either select **File** > **Print** or click the **Print** button

on the main CHEMCAD toolbar. Follow the prompts for your printer to complete the printing process.

16. To close CHEMCAD, select **File** > **Close**, or click the **Close** button in the upper right corner of the CHEMCAD window. Click **Yes** at the message asking whether you want to exit CHEMCAD, then click **Yes** again to save changes to the simulation.

CC-THERM Tutorial

This tutorial walks you through the rating of a heat exchanger. The example you'll work with is the condensate stabilizer example described in the CC-STEADY STATE tutorial, which looks like this:



While it's recommended that a new CHEMCAD user build this simulation from the ground up to gain proficiency with the software, a ready-made example called **CHEMCAD Tutorial.CC6** is also available. This file is located by default in the directory called **My Documents\My Simulations\Examples\Tutorials**.

Your objective is to rate the first heat exchanger in this flowsheet. The equipment you're working with is a countercurrent gas/gas heat exchanger with the following geometry and dimensions:

- TEMA class = R
- TEMA type = BEM
- Fouling factors = 0.001 both sides
- Shell inside diameter = 27″
- Number of tubes = 646
- Tube outside diameter = 0.75″
- Tube wall thickness = 0.065″
- Tube length = 20′
- Tube pattern = rotated triangular (60°)
- Tube pitch = 0.9375″
- Baffles: 10, equally spaced
- Baffle type = single segmental
- Baffle cut = 35% (diameter)
- Impingement plate present
- Shell-side nozzles = one, 12″

- Tube-side nozzles = one, 12″
- Baffle to shell I.D. clearance = 0.3125″ (diameter)
- Shell I.D. to OTL clearance = 0.35433″ (diameter)
- Tube to baffle hole clearance = 0.035″ (diameter)
- Space at top of bundle = 2.8″
- Carbon steel tubes; all other materials A-285-C
- 5 rows per sealing strip

Overview of the Heat Exchanger Sizing Process

The CC-THERM module enables you to generate heat curves and specify heat exchangers. This process involves the following steps:

1. Identify the tube-side stream.
2. Generate and finalize the heat curve and properties on both sides of the exchanger.
3. Define general information about the exchanger.
4. Specify any desired tube data.
5. Specify any desired shell data.
6. Specify any desired baffle data.
7. Specify any desired nozzle data.
8. Specify any desired specific clearances.
9. Specify the materials used in the construction of the heat exchanger.
10. Specify any desired miscellaneous data.
11. Run the sizing calculations.
12. Review results and create plots as needed.

Identify the Tube-side Stream

Once the simulation is complete in CC-STEADY STATE, you can start sizing the first heat exchanger by identifying the tube-side stream:

1. Click on the first heat exchanger icon and then select **Sizing** > **Heat Exchangers** > **Shell & Tube**.
2. A message box prompts you to select a stream entering the exchanger's tube side. Click **OK** to continue.
3. At the Select Streams dialog box, either type **1** or click stream 1 on the flowsheet, then click **OK**.

4. CC-THERM displays data for all four streams around the exchanger in a separate report window. Review or print the data as needed and then close the report window.

Generate the Heat Curve

Once the tube-side stream is identified, CC-THERM prompts you through the setup of the heat curve. The Heat Curve Parameters dialog box displays as soon as you close the report from the previous step.

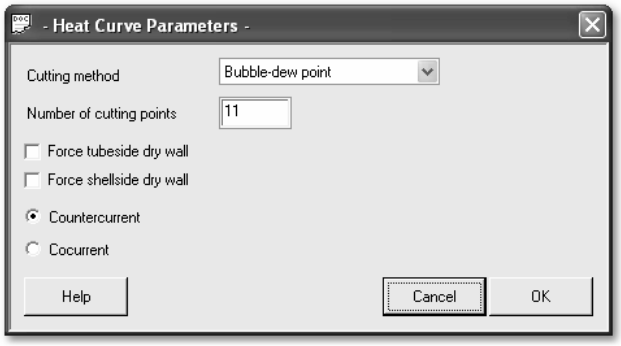


Figure 11-21: The Heat Curve Parameters dialog box

To account for the change in physical properties across the heat exchanger, CC-THERM divides the analysis into zones. These zones are thermodynamic segments based on equal temperature changes or equal enthalpy increments. There are two options to choose from:

- **Equal enthalpy:** Increments of equal enthalpy change
- **Bubble-dew point:** Increments of equal enthalpy change between the dew and bubble points, with separate zones for superheating and subcooling if present

The default setting is the bubble-dew point option. For either segmentation method, you can also decide how many zones to calculate for the exchanger. The more zones you specify, the more accurate the calculations will be, but calculations will also be slower. The industry standard is 10 zones (11 points), which is the default entry here, but you can select any number by making an entry in the **Number of cutting points** field. Bear in mind that the number of points equals the number of zones plus one.

For this tutorial, leave all the default settings and click **OK** to continue. CC-THERM calculates the 11 points needed for the heat curve and displays a plot like the one shown in Figure 11-22.

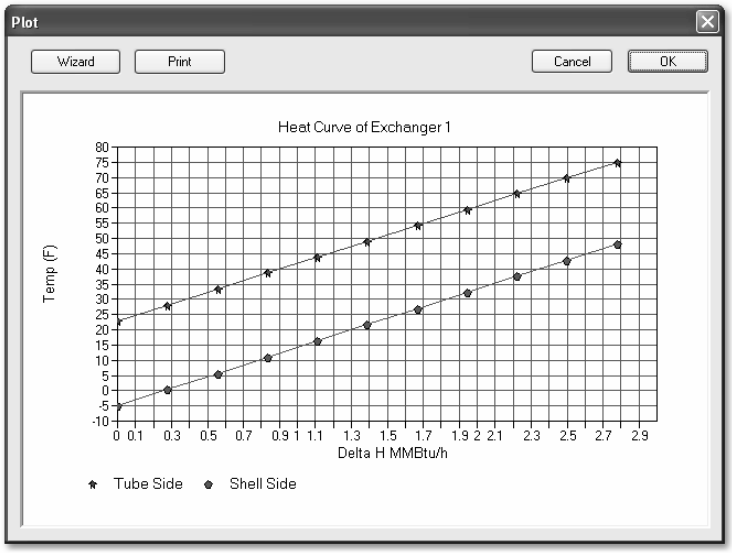


Figure 11-22: Heat curve plot for first heat exchanger

This plot enables you to inspect the calculated heat curve for any obvious problems in the setup of the analysis. Click **OK** to close this window and continue.

Define General Specifications

The next dialog box to appear is called General Specifications. Here, you can provide basic information governing heat exchanger calculations, such as process type, allowable pressure drop, fouling factor, TEMA class and type, and so forth.

This dialog box has two tabs, and most of the fields on both tabs have default settings. The tab that initially displays is called **General Information**, and it includes the following settings:

- **Calculation mode:** This entry determines whether you are designing or rating a heat exchanger. Use the default setting of **Rating**.
- **TEMA class/standard:** This entry specifies the exchanger's TEMA class, which is primarily a function of its mechanical details. Use the default setting of **TEMA R**.
- **Orientation:** This entry specifies whether the exchanger is mounted horizontally or vertically. Use the default setting of **Horizontal**.
- **TEMA front end head**, **TEMA shell type**, and **TEMA rear end head:** To establish the basic configuration of the exchanger, you must define these characteristics of the exchanger according to TEMA designations. The simplest and most common kind of exchanger is a fixed tubesheet, or BEM, TEMA type. Select **B - Bonnet** for the front head, **E -One Pass** for the shell type, and **M - Fixed Tubesheet (B head)** for the rear head.
- **Process type:** In some cases, you must identify the process type, for example in the case of pool boiling or falling-film condensation. In this case, use the

default selection of **Sensible Flow** for both tube side and shell side, as there is no phase change on either side of the exchanger.

- **Fouling factor** - To allow for fouling on the inside and outside of the tube, you can enter fouling factors. Use the default setting of **0.001** (English units) on both sides.

On the **Modeling Methods** tab, you can select the formulas to be used in certain aspects of the heat exchanger calculations. For the purposes of this tutorial, use the program's default selections. Click **OK** to continue.

Set Tube Specifications

The Tube Specifications dialog box now appears, populated with default entries in all fields.

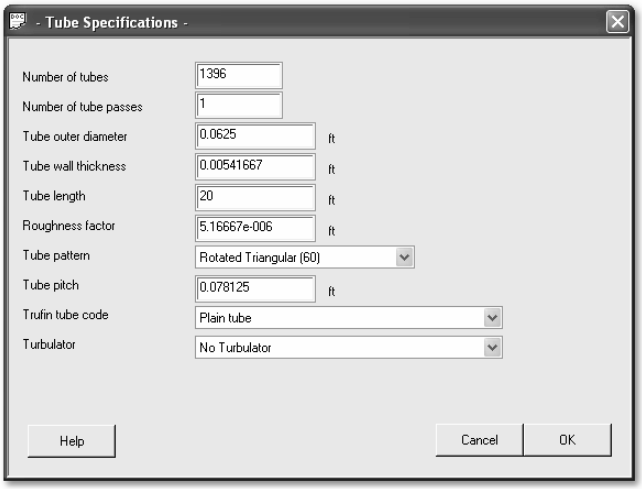


Figure 11-23: The Tube Specifications dialog box

Enter **646** in the **Number of tubes** field and click **OK** to continue.

Set Shell Specifications

The next dialog box to appear is called Shell Specifications.

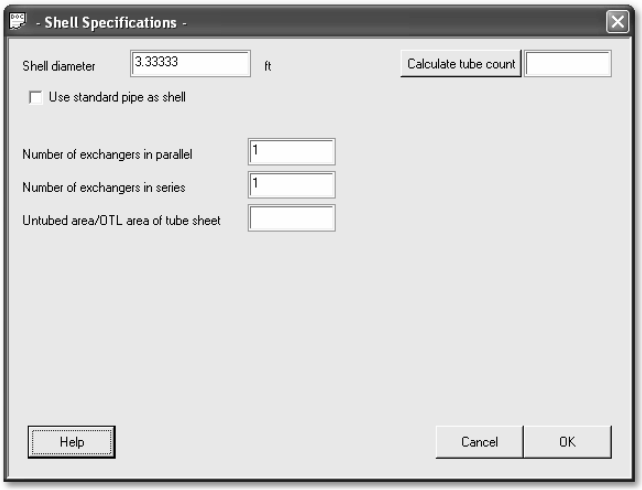


Figure 11-24: The Shell Specifications dialog box

The only value that you need to specify here is the shell diameter. Unless you check the **Use standard pipe as shell** box, CC-THERM assumes that the value entered here is the actual shell inside diameter. Type **2.25** (the equivalent in feet to 27″) in the **Shell diameter** field and then click **OK** to continue.

Note: The CHEMCAD suite has a handy built-in conversion feature that can help when input fields require a different unit of measure than the data you have. Place your cursor in any numeric data entry field, and then press **[F6]** to bring up a dialog box that offers conversion units relevant to the selected field. Type the value you have in the appropriate field and press **[ENTER]** to convert to other units. Verify the results of the conversion and then click **OK**. CHEMCAD automatically selects the appropriate units for the field and enters that converted value.

Set Baffle Specifications

The Baffle Specifications dialog box displays next.

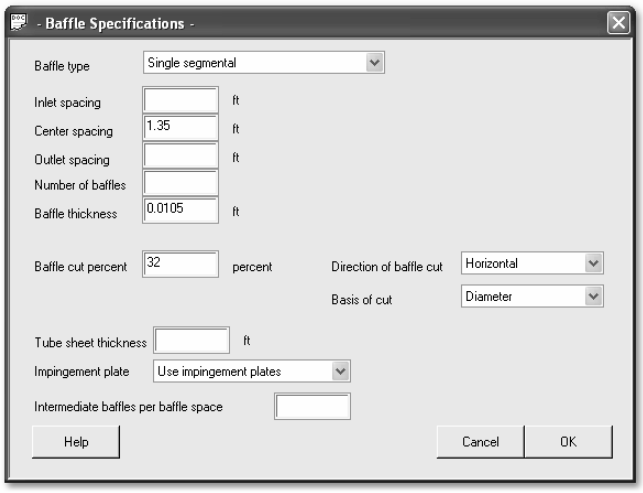


Figure 11-25: The Baffle Specifications dialog box

Most of the default entries here are appropriate for this example; you do, however, need to specify the baffle spacing and baffle cut.

Baffle Spacing

All that you know for the purposes of baffle spacing is that there are 10 baffles equally spaced. Erase any default values for spacing and enter **10** in the **Number of baffles** field. CC-THERM will calculate equal spacing for the baffles.

Baffle Cut Percent

The baffle cut percent can be based either on diameter or on area. The **Basis of cut** field identifies the basis for the specified cut; use the default setting of **Diameter**, and enter **35** in the **Baffle cut percent** field. Click **OK** to continue.

Set Nozzle Specifications

The Nozzle Specifications dialog box now appears.

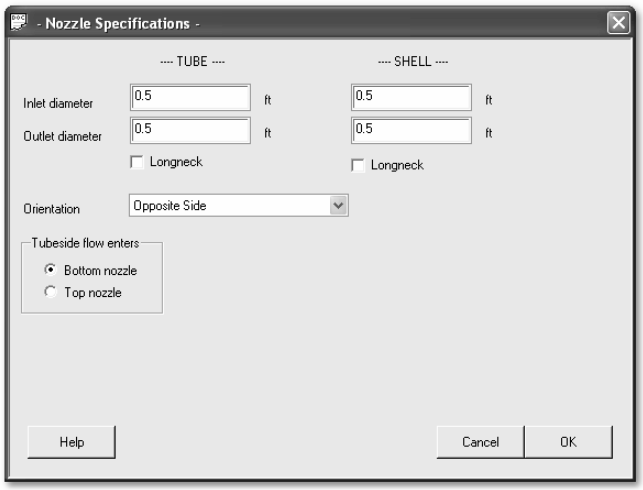


Figure 11-26: The Nozzle Specifications dialog box

The default entries are acceptable for this example, so you only need to enter the inside diameter for the inlet and outlet nozzles on both the tube and shell sides. All of these nozzles have 1′ internal diameters.

Enter **1** in each of the four fields at the top of the dialog box, then click **OK** to continue.

Set Clearance Specifications

You will now see the Clearance Specifications dialog box.

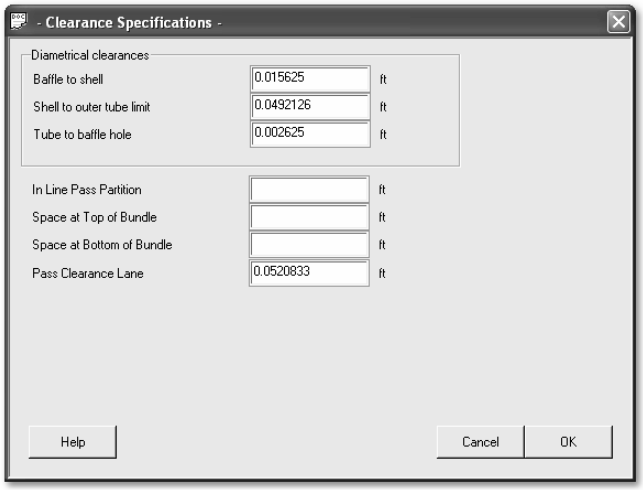


Figure 11-27: The Clearance Specifications dialog box

CC-THERM always defaults to TEMA clearances, so normally no entry is required in this dialog box. In this case, the clearances are known, so you should enter them in the event they do not conform exactly to TEMA. You can use the **[F6]** feature noted earlier in this tutorial to convert the given clearances from inches to feet.

Also, because there is an impingement plate, you need to enter the space at the top of the bundle. Type **0.233333** in the **Space at Top of Bundle** field and then click **OK** to continue.

Set Material Specifications

The next dialog box to appear is called Material Specifications.

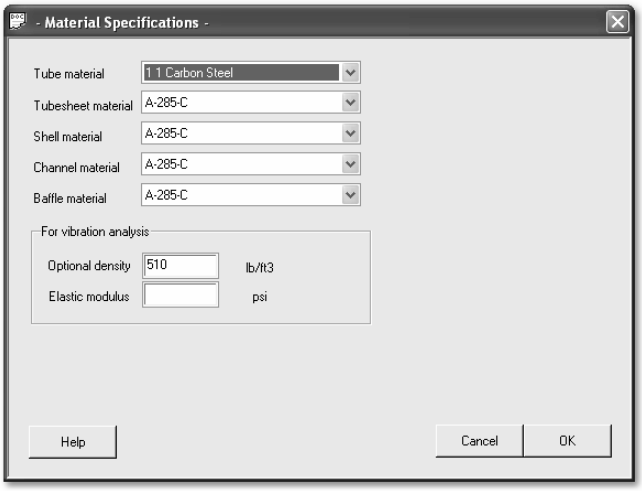


Figure 11-28: The Material Specifications dialog box

Here, you can specify the materials of construction for the heat exchanger. For this example, use the default entries: carbon steel for the tubes and A-285-C for all other materials. Click **OK** to continue

Set Miscellaneous Specifications

The last dialog box to appear is called Miscellaneous Specifications.

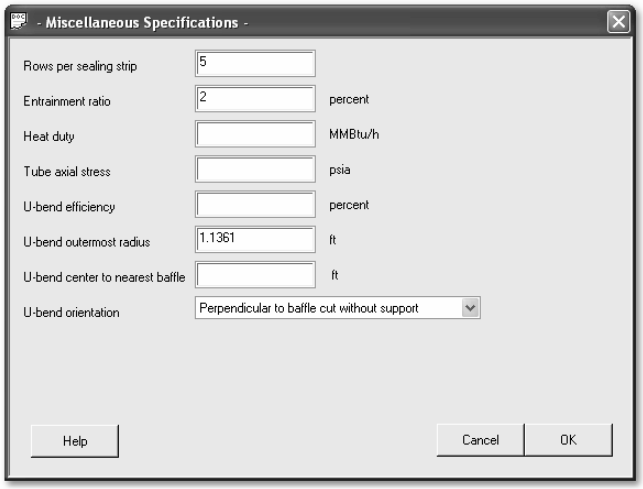


Figure 11-29: The Miscellaneous Specifications dialog box

The only field that is important to this example is **Rows per Sealing Strip**. The default entry of **5** is what the example calls for, so leave the dialog box as it is and click **OK** to continue.

Run Sizing Calculations

Now that you have specified heat exchanger data in all of the required dialog boxes, the Shell and Tube Exchanger menu appears. Note that this menu is what you will

see if you return to shell and tube sizing for this exchanger at any time after this initial specification.

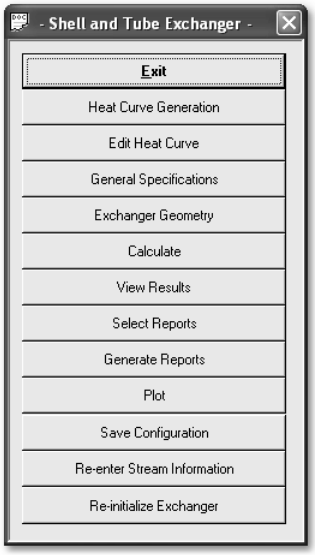


Figure 11-30: The Shell and Tube Exchanger menu

Click the **Calculate** button on the menu. The calculation will run very fast, showing runtime messages on the status bar and then returning you to the Shell and Tube Exchanger menu.

Review Results and Create Plots

Now that calculations are complete, you can click the **View Results** button to see the result of the heat exchanger calculations. The View Results menu will appear.

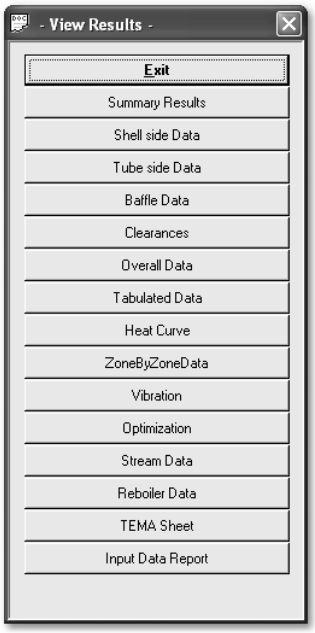


Figure 11-31: The View Results menu

Click any of these buttons to view various reports on everything from baffle parameters to vibration analysis. When you select a report, the data displays in a

separate window, which you can review or print and then close. To return to the Shell and Tube Exchanger menu at any time, click the **Exit** button.

You can also display results graphically by clicking **Plot**. This opens the Plot menu, from which you can select a variety of zone-by-zone graphs.

Figure 11-32: The Plot menu

These plots open in a plot window, just like the heat curve plot that you we saw at the beginning of this tutorial. When you click **OK** to close any plot, you will return to the Shell and Tube Exchanger menu.

You can also print tabulated, hard-copy reports using the **Select Reports** and **Generate Reports** options on the Shell and Tube Exchanger menu. First, click **Select Reports** to bring up the Report Selection dialog box.

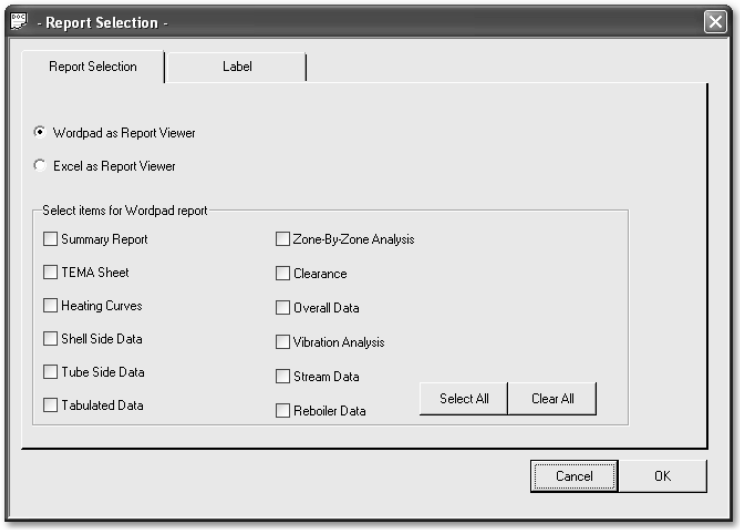


Figure 11-33: The Report Selection dialog box

Select either WordPad or Excel as your report viewer, and check the boxes for the reports that you want to generate. Click **OK** to return to the Shell and Tube Exchanger menu, then click **Generate Reports**. All of the reports that you selected will be generated and displayed using the viewer that you chose.

You can now review or print the report; when you close the report window, you will return to the Shell and Tube Exchanger menu. Click **Exit** to close the menu, then click **Yes** when asked whether you want to save your changes.

CC-BATCH Tutorial

This tutorial walks you through the process of using CC-BATCH to simulate a batch distillation column.

Description of the Problem

The simulation you will create is a five-step batch distillation campaign, as illustrated in Figure 11-34. The objective is to separate 100 lb•mol of mixed propane, butane, pentane, and hexane into three separate tanks, producing 99% pure butane.

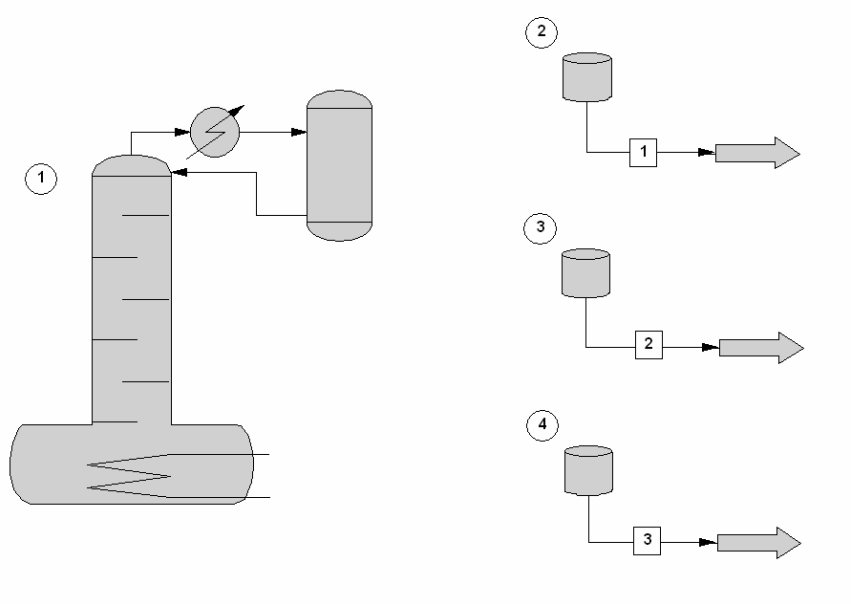


Figure 11-34: The batch distillation flowsheet

The following are detailed specifications for this problem:

Thermodynamic Selections	Column Specifications
• **K-value:** Peng-Robinson • **Enthalpy:** Peng-Robinson	• **No. of internal stages:** 8 • **No. of operations:** 5 • **Internal stage holdup:** 0.01 ft^3 • **Condenser holdup:** 0.1 ft^3 • **Condenser pressure:** 14.7 psia • **Column pressure drop:** 2 psia

Initial Charge Conditions	Initial Charge Composition (mole frac)
• **Temperature:** Calculated • **Pressure:** 16.7 psia • **Vapor Fraction:** 0 at bubble point • **Total amount of charge:** 100 lb•mol	• **Propane:** 0.1 • **N-Butane:** 0.3 • **N-Pentane:** 0.1 • **N-Hexane:** 0.5

Operating Step 1

- **Purpose:** Propane removal
- **Reflux ratio:** 5
- **Distillate molar flow rate:** 2
- **Stop when:** Distillate mole fraction of N-Butane is 0.2
- **Materials to be added at start:** None

Operating Step 2

- **Purpose:** Propane removal
- **Reflux ratio:** 20
- **Distillate molar flow rate:** 2
- **Stop when:** Distillate mole fraction of N-Butane is 0.985
- **Materials to be added at start:** None

Operating Step 3

- **Purpose:** Butane production
- **Reflux ratio:** 25
- **Distillate molar flow rate:** 2
- **Stop when:** Accumulator mole fraction of N-Butane is 0.99
- **Materials to be added at start:** 20 lb•mol of mole fraction 40% N-Butane/60% N-Hexane, at its bubble point at 16.7 psia

Operating Step 4

- **Purpose:** Pentane removal
- **Reflux ratio:** 15
- **Distillate molar flow rate:** 2
- **Stop when:** Distillate mole fraction of N-Hexane is 0.2
- **Materials to be added at start:** None

Operating Step 5

- **Purpose:** Pentane removal
- **Reflux ratio:** 25
- **Distillate molar flow rate:** 2
- **Stop when:** Bottom mole fraction of N-Hexane is 0.9998
- **Materials to be added at start:** None

Overview of the Batch Distillation Process

The process of building the flowsheet and simulating the batch distillation involves the following steps:

1. Create a new simulation.
2. Select engineering units.
3. Draw the flowsheet.
4. Select the components.
5. Select thermodynamic options.

6. Specify pot charge.
7. Specify the distillation column.
8. Define operating steps.
9. Run the simulation.
10. Review the results and print as needed.

Creating a New Simulation

Start by creating a new simulation and giving it a name.

To do this, launch CHEMCAD and then Select **File** > **Save** to open the Save As dialog box. Navigate to the directory where you want to store the simulation (try My Simulations, located under My Documents) and give your simulation a name, leaving the type as **CHEMCAD 6 (*.cc6)**. Then click **Save** to create the file and return to the main CHEMCAD window.

Selecting Engineering Units

Select **Format** > **Engineering Units** to open the Engineering Unit Selection dialog box.

The **English** units option is the default and is currently highlighted. To change the engineering units system, you would click the **Alt SI**, **SI**, or **Metric** button; you could then change any of the individual units as well. For this tutorial, you will use English units, so click **Cancel** to exit this dialog box without making changes.

Drawing the Flowsheet

As described in Chapter 5, creating a flowsheet is a matter of placing UnitOp icons on the screen, connecting them with streams, and then adding various graphical objects to enhance the drawing.

Placing UnitOps

Begin by placing the Batch Column unit on the screen.

1. On the All UnitOps palette, click the **Batch column** tool (see Figure 11-35) and then click in the main CHEMCAD workspace. The batch column icon appears where you clicked.

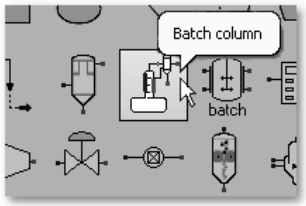


Figure 11-35: The icon representing a batch column

2. Click the **Tank** tool (see Figure 11-36). On the workspace, click to the right of the batch column to place a tank icon. Then click just below the first tank, and

click again below the second tank. When you have placed all three tanks on the flowsheet, right-click to deactivate the **Tank** tool.

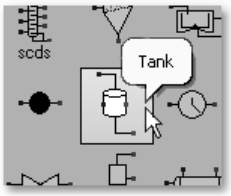


Figure 11-36: The tank icon

3. Click the **Product** tool (see Figure 11-37) and in similar fashion, place three product arrows on the flowsheet, each one below and to the right of a tank icon. Right-click to deactivate the **Product** tool.

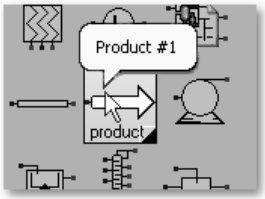


Figure 11-37: The product icon

Drawing Streams

Now that all of the UnitOps are in place, select the **Stream** tool and connect each tank's outlet to the nearest product arrow. These are the only streams that you need for this tutorial.

Note: In this simulation, the batch distillation column transfers products to the tanks based upon batch operation parameters that you provide. Stream connections between the column and the tanks are not necessary, and are ambiguous given the dynamic nature of such streams.

Remember that each stream must start at a red outlet point on the upstream UnitOp, and end at a blue inlet point on the downstream UnitOp. To avoid having to re-select the **Stream** tool each time, make sure that as soon as you click to complete one stream, you move the cursor to the next location and click to start the next stream.

As you draw streams, CHEMCAD assigns stream IDs, just as it assigned UnitOp IDs when you created those items. The labels for stream IDs are displayed in squares, to distinguish them from the UnitOp IDs displayed in circles.

At this point, the flowsheet should look similar to Figure 11-34.

Selecting Components

Now you need to identify the components to be used in this simulation. Start by selecting **Thermophysical** > **Select Components**.

For this example, you'll choose components from the standard CHEMCAD database. In the Select Components dialog box, find and add each needed component.

1. Hold down the **[CTRL]** key on your keyboard as you click each of the following components in turn:
   - 4 Propane
   - 6 N-Butane
   - 8 N-Pentane
   - 10 N-Hexane
2. Click the right arrow button, located to the right of the *Available Components* area, to add all of the selected components to your simulation. The Select Components dialog box should now look like Figure 11-38.

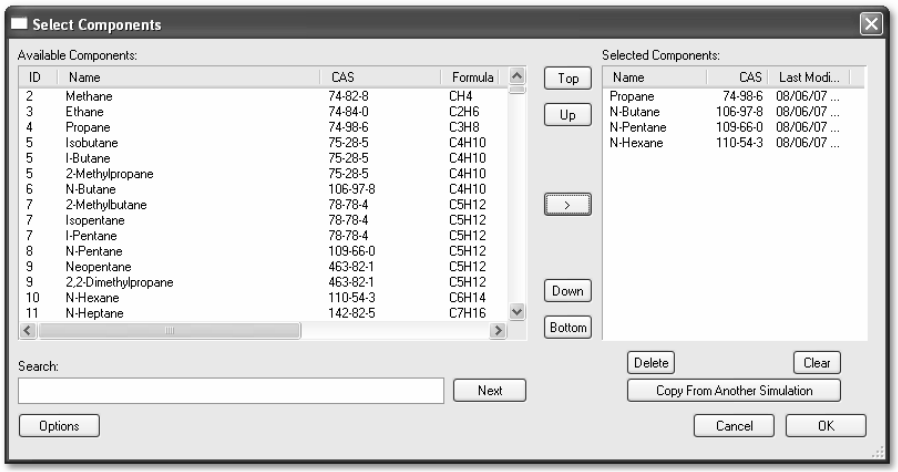


Figure 11-38: The completed Select Components dialog box

3. Save your component selections by clicking **OK**.

Selecting Thermodynamic Options

As soon as you have finished component selection, the Thermodynamics Wizard appears. This tool can suggest thermodynamics options to use with this simulation.

CHEMCAD's Thermodynamics Wizard works like this:

1. First, it looks at the component list and decides what general type of model is required, i.e., equation-of-state, activity model, etc.
2. Second, it looks at temperature and pressure ranges that you provide and decides which equation within a given category is best at the limits of those ranges.

3. If the method is an activity model, the program then looks at the BIP database to see which model has the most data sets for the current problem. It then calculates the fractional completeness of the BIP matrix. If that fraction is greater than the BIP threshold parameter, it uses the chosen activity method; if not, it uses UNIFAC.

The Thermodynamics Wizard is no replacement for engineering judgment. This tool uses an algorithm based on general rules, and is therefore fallible. The suggested model might not always be the best model for the system.

Selecting thermodynamic options basically means selecting a model or method for calculating vapor-liquid (or vapor-liquid-liquid) phase equilibrium (called the *K-value option*) and selecting a method or model for calculating the heat balance (called the *enthalpy option*). The commands for these selections are located on the Thermophysical menu.

CHEMCAD has a library of dozens of K-value models with a variety of options and about 12 enthalpy models. Making the proper selection from these libraries can sometimes be difficult. For the purposes of this tutorial, assume that you want to use the Peng-Robinson method for both the K-value and enthalpy calculations. Follow these steps to select your thermophysical options:

1. Accept the default temperature and pressure ranges in the Thermodynamics Wizard and click **OK**.
2. Click **OK** again to accept the wizard's suggested method of SRK.
3. When the Thermodynamic Settings dialog box opens, find the Global K-Value Option selection, in the upper left corner of the K-Value Models tab. The current setting is **SRK**, but for the purposes of the tutorial, you'll need to select the Peng-Robinson model. Click the down arrow at the right end of the selection box to view a long list of K-value choices, then click **Peng-Robinson**.

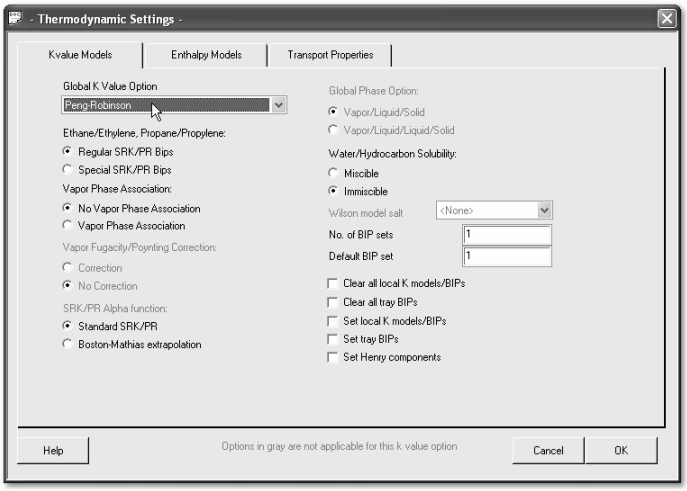


Figure 11-39: The new K-value selection in the Thermodynamic Settings dialog box

4. Now click the **Enthalpy Models** tab. The Peng-Robinson method has already been entered as the Global Enthalpy Options selection; this was done automatically because you chose Peng-Robinson as your K-value method. While you do have the option to override this choice, in this case you'll need to keep the Peng-Robinson model; leave all settings as they are and click **OK** to return to the main CHEMCAD workspace.

For the purpose of this tutorial, the thermodynamic selections are now complete.

Note: While you are not required to use the Thermodynamics Wizard, you should know how to use it, if only as a starting point for your simulations. You can revisit the wizard at any time by selecting **Thermophysical** > **Thermodynamics Wizard**.

Specifying Pot Charge

Now that you have thermodynamics and components defined for this simulation, and you have a batch column in the flowsheet, you can define the pot charge for the column.

You will specify the pot charge according to the following rules:

- The **Temp F**, **Pres psia**, **Vapor Fraction**, and **Enthalpy MMBtu/h** fields are the *thermodynamic properties* of the charge. According to the Gibbs Phase Rule, once a mixture's composition is given, specifying any two of these four thermodynamic properties will define the other two. As such, defining the composition, temperature, and pressure for a mixture uniquely defines its vapor fraction and enthalpy. Alternatively, defining the composition, pressure, and enthalpy will uniquely define the mixture's temperature and vapor fraction.

  Since enthalpies are calculated relative to a datum, the calculation of any given enthalpy is an involved process which is prone to errors. For this reason, CHEMCAD does not permit you to enter enthalpy as a constraint.

  In addition to defining the pot composition, you must define exactly two of the following properties: temperature, pressure, and vapor fraction. The two variables that you specify will display as red text, while the third variable and the value enthalpy will be displayed in black when you flash the charge.

- The **Total flow unit** and **Comp unit** fields work together to provide a variety of ways to define charge composition. If the selected comp unit is mole, mass, or volume fraction (either globally or locally), then the **Total flow unit** selection is available. If the selected comp unit is an amount option, then the total charge becomes the sum of the component quantities, and the **Total flow unit** selection is not available.

- If the **Comp unit** field selection is an amount unit (as opposed to a fractional unit), then the component charge values are automatically added as you enter them. The current sum is displayed in the **Total flow** field.

- You can click the **Flash** button at any time to perform a flash calculation using the currently specified composition and thermodynamic properties. This enables you to obtain flash calculations quickly and without leaving the dialog box.
- Fractions that do not add up to 1.0 are automatically normalized when you either click **Flash** or exit the dialog box.

With these rules and behaviors in mind, enter the data for your pot charge:

1. Double-click the batch column to open the Edit Batch Charge dialog box.

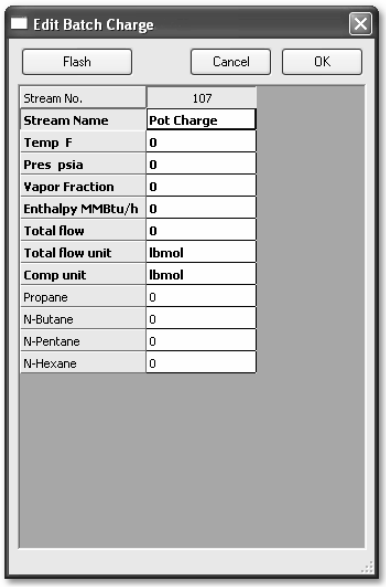


Figure 11-40: The Edit Batch Charge dialog box

2. In the **Pres psia** field, type **16.7**, then press **[TAB]** and type **0** in the **Vapor Fraction** field.

Note: It's important that you actually type a **0** over the existing **0** entry in the **Vapor Fraction** field. This tells CC-BATCH that you are choosing to specify a vapor fraction.

3. In the **Comp unit** field, select **mole frac**. You can now type a value of **100** in the **Total flow** field.
4. Type **0.1** in the **Propane** field, and then in similar fashion, type the following numbers in the corresponding fields:
   - N-Butane: **0.3**
   - N-Pentane: **0.1**
   - N-Hexane: **0.5**
5. Click **OK** to save this charge information and continue.

Specifying the Distillation Column

When you have specified the pot charge, CC-BATCH displays the Batch Distillation Column dialog box.

Figure 11-41: The Batch Distillation Column dialog box

Make the following entries on the **General** tab of this dialog box:

- Number of stages: **8**
- Number of operation steps: **5**
- Stage holdup: **.01**
- Condenser holdup: **1**
- Cond pressure: **14.7**
- Colm pres drop: **2**

When you have entered these parameters, click **OK** to save the data and continue.

Defining the Operating Steps

When you have completed the initial column specification, the Batch Operation Parameters dialog box appears.

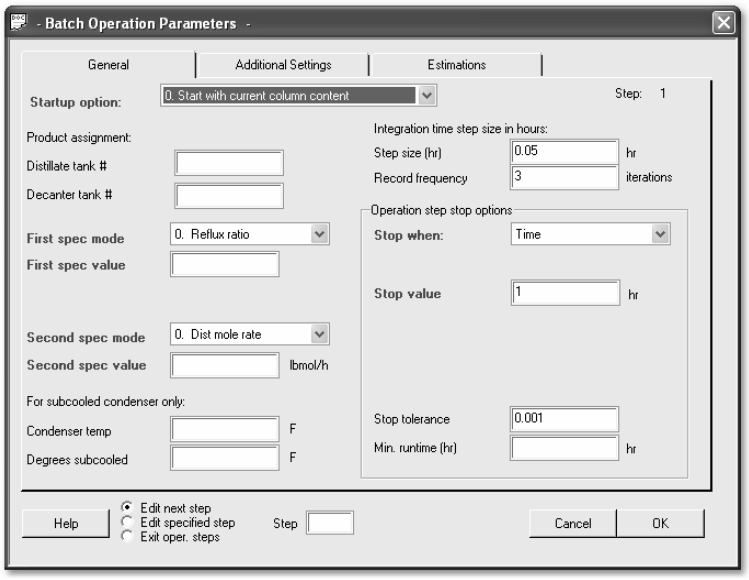


Figure 11-42: The Batch Operation Parameters dialog box

In this dialog box, you'll define the parameters for each operating step of the batch campaign. Before you begin, you need to understand how CC-BATCH handles tank assignments.

The **Product assignment** fields identify the accumulator to which a product or decant stream will be sent. You can use this option even if you do not place tanks on the flowsheet; simply designating a UnitOp ID number is sufficient. In this case, it's important that you designate a UnitOp ID that is not already in use.

Since CC-BATCH permits vapor-liquid-liquid distillation, there may be two liquid phases in the condenser, possibly giving rise to decanting of one phase or the other. The **Distillate Tank** # field entry represents the tank that accumulates the distillate. The **Decanter Tank** # field entry represents the tank that accumulates the decanted liquid, if any.

Operating Step 1

For operating step 1, make the following entries in the Batch Operation Parameters dialog box:

- Change the **Startup option** field to **1 Start with total reflux**.
- In the *Product assignment* area, enter **2** in the **Distillate tank** # field.
- In the **First spec value** field, enter **5** as the value of the reflux ratio.
- In the **Second spec value** field, enter **2**.

- In the *Operation step stop options* area, set the **Stop when** option to **Distillate**, set the **Measured variable** option to **Mole fraction**, and enter **0.2** in the **Stop value** field. In the **Component** field that now appears, select **2 N-Butane**.
- In the **Min. runtime** field, enter **0.5**.

When you have made these entries, click **OK** to move on to the next operating step.

Operating Step 2

For operating step 2, make the following entries in the Batch Operation Parameters dialog box:

- Enter **2** in the **Distillate tank #** field.
- Enter **20** in the **First spec value** field and **2** in the **Second spec value** field.
- Stop the operation when the mole fraction of N-Butane in the distillate is **0.985**.

When you have made these entries, click **OK** to move on to the next operating step.

Operating Step 3

Follow these steps for operating step 3:

1. Make the following entries in the Batch Operation Parameters dialog box:
   - Enter **3** in the **Distillate tank #** field.
   - Enter **25** in the **First spec value** field and **2** in the **Second spec value** field.
   - Stop the operation when the mole fraction of N-Butane in the accumulator is **0.99**.
2. Click the **Additional Settings** tab. Here you will specify the addition of 20 moles of mixture to the pot, with a composition of 40% butane and 60% hexane. Check the **Add material to pot** box and then click **OK** to bring up the Edit Batch Charge dialog box.
3. In the **Pres psia** field, type **16.7**, then press **[TAB]** and type **0** in the **Vapor Fraction** field.
4. Enter the following composition settings:
   - Set the **Comp unit** field to **mole frac**.
   - Enter **0.6** in the **N-Butane** field.
   - Enter **0.4** in the **N-Hexane** field.
   - Enter **20** in the **Total flow** field.
5. Click **OK** to continue to the next operating step.

Operating Step 4

For operating step 4, make the following entries in the Batch Operation Parameters dialog box:

- Enter **4** in the **Distillate tank #** field.
- Enter **15** in the **First spec value** field and **2** in the **Second spec value** field.
- Stop the operation when the mole fraction of N-Hexane in the distillate is **0.2**.
- In the **Min. runtime** field, enter **0.5**.

When you have made these entries, click **OK** to move on to the final operating step.

Operating Step 5

For operating step 5, make the following entries in the Batch Operation Parameters dialog box:

- Enter **4** in the **Distillate tank #** field.
- Enter **25** in the **First spec value** field and **2** in the **Second spec value** field.
- Stop the operation when the mole fraction of N-Hexane in the residual charge at the bottom of the column is **0.9998**.
- In the **Min. runtime** field, enter **0.5**.

When you have made these entries, click **OK** to continue.

The Run Time Information Dialog Box

At the completion of the last operating step, the Run Time Information dialog box displays. Here, you can choose which variables will be plotted when you run the simulation.

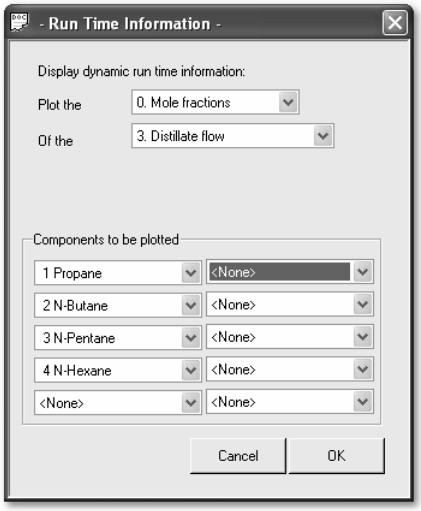


Figure 11-43: The Run Time Information dialog box

For this example, the default display—a plot of distillate mole fractions for all four components—is what you want, so click **OK** to bring up the Batch Distillation menu.

Figure 11-44: The Batch Distillation menu

This menu provides access to the entry screens for all defined operation steps, as well as options for inserting, deleting, and copying operation steps. You might want to review the operating steps and verify your entries before running the simulation. When you are finished, click the **Exit** button to close the menu.

Running the Simulation

To run the simulation, click the **Run All** toolbar button. CC-BATCH first checks the input data for errors or omissions. You may see the following types of messages:

- **Error messages** must be fixed before the simulation can proceed. Under-specification of the batch column would be an example of this type of error.
- **Warning messages** are usually input omissions, which may or may not cause problems upon execution. These are non-fatal errors that do not necessarily need to be corrected prior to simulation.

Assuming that you correctly specified the pot charge and subsequent operation steps, you should see no messages; the program will proceed directly to the calculation.

You will see the distillate mole fractions plotted on the screen in a plot window. Each time the program proceeds to the next operating step, a new plot window will open, along with a new tab at the bottom of the main CHEMCAD workspace. During the run, only the current step's plot is visible. When the simulation is finished, the dynamic plot will quit scrolling and a *Run finished* message will appear at the far left end of the CHEMCAD status bar.

After the run, you can view the plot for a particular operating step by clicking the corresponding tab at the bottom of the CHEMCAD workspace. To close any plot's tab, click the **Close** button (marked with an **X**) on the tab. To close all of the plot tabs at the same time, select **Window** > **Close All Charts**.

Reviewing and Printing Results

Once the simulation is complete, you can review the results interactively before printing a hard copy. The commands needed to do this are located in the **Report** and **Plot** menus.

Plotting the Results

For batch calculations, the most convenient way to examine the output is to plot the results. To do this, click your batch column UnitOp and then select **Plot** > **Dynamic Plots** > **Batch Column History**.

This brings up the Batch Column Plots dialog box. From here, you can generate a plot that encompasses the entire campaign. For example, you can follow these steps to plot distillate mole fractions across all operating steps:

1. In the **Plot variable** field, select the **0 Mole fractions** option.
2. In the **Of the** field, select the **3 Distillate** option.
3. In the *Components to plot* area, use the first four fields to select the four components found in the distillate.

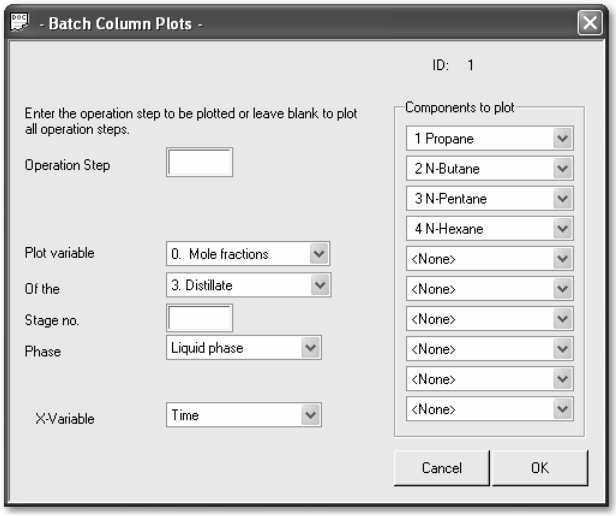


Figure 11-45: The completed Batch Column Plots dialog box

4. Click **OK** to view the composite plot, which should resemble Figure 11-46.

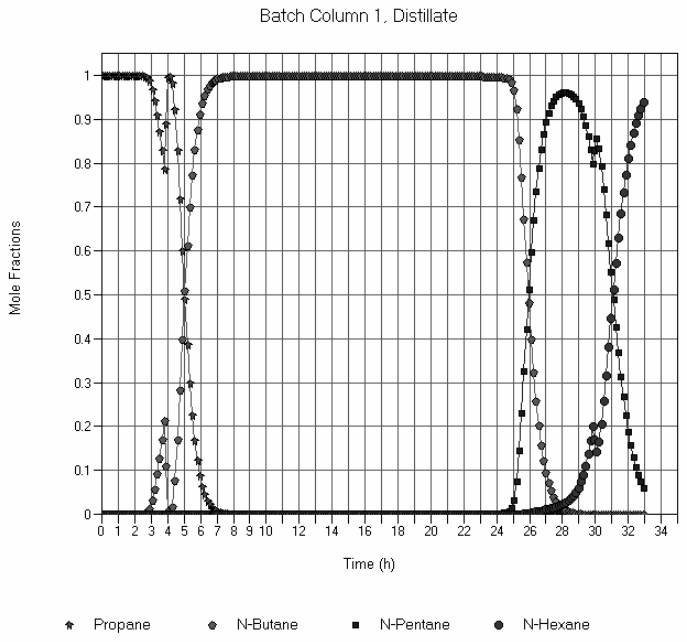


Figure 11-46: Composite plot showing composition of distillate over time

Review or print the results as needed, and then close the plot tab to return to the simulation.

Generating Text Reports

You can also view certain batch results in tabular format. To do this, select **Report** > **Batch Results**. A summary of the results of this simulation displays in a separate window. Review or print the results as needed, and then close the report window to return to the main CHEMCAD window.

Generating a Full Report

The Report menu offers a broad array of text reports, as described in Chapter 8, *Output and Reports*. For the purpose of this tutorial, assume that you want to view and print out a report with the following information:

- Operating step results
- Batch column history
- Final batch column holdup

Because you want a report with a broad range of information about your simulation, use the Consolidated Report option.

1. Select **Report** > **Consolidated Report** to bring up the Consolidated Report menu.
2. Click **Batch/Dynamic Results** to open the Batch/Dynamic Options dialog box. Select the first three options **Print operation results**, **Print history**, and **Print final holdups**.

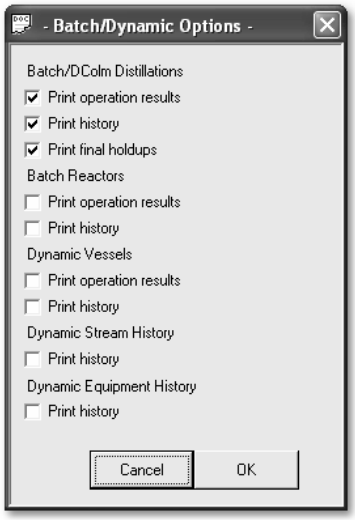


Figure 11-47: The Batch/Dynamic Options dialog box

3. Click **OK** to return to the Consolidated Report menu.
4. To generate the report, click **Calculate and Give Results**. The report displays in a separate window, with a format suitable for printing. You can edit, save, and print the report as needed.
5. When you finish reviewing and working with the report, close the report window to return to the main CHEMCAD workspace.

Piping Tutorial

A piping network represents the flow of fluids through several pieces of equipment. If sufficient variables (flow rate and pressure) are specified on the piping network, CHEMCAD calculates the unknown variables.

For fluid flow through equipment, flow rate may be calculated as a function of the inlet and outlet pressure. If you know any two of these three variables, CHEMCAD can calculate the third.

In this tutorial, you will work with CHEMCAD's piping features. You will perform control valve and orifice sizing and rating; simulate complex piping networks; use feedback controllers; calculate NPSH; and make appropriate equipment selections.

Control Valve Sizing Example

This portion of the piping tutorial covers control valve sizing, control valves, and the use of nodes.

Problem Statement

For this part of the tutorial, reference the flowsheet shown in Figure 11-48. This example is called **Example 1**, and it's located in the **My Simulations\Examples\Piping** folder.

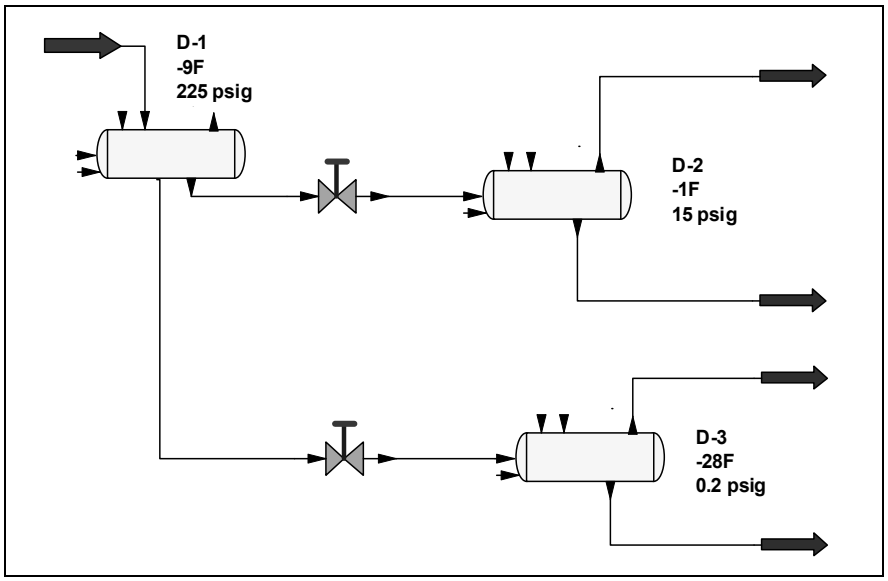


Figure 11-48: Diagram of control valve sizing example

You need to size control valves for handling a flow of 113,000 lb/hr of liquid ammonia in each line coming from vessel D-1. You must select properly-sized valves and then determine the percent open for each valve at the rated service.

To perform the initial sizing, all you need are streams with the correct properties (see Figure 11-49). It is not necessary to model the tanks.

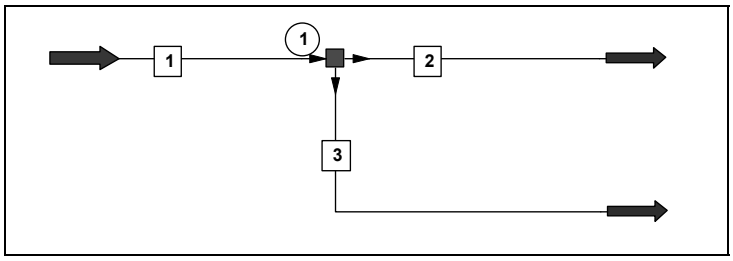


Figure 11-49: Streams for initial sizing

All three streams in Figure 11-49 are at the inlet conditions of -9° F and 225 psig. The divider splits the 226,000 lb/hr flow into two equal flows of 113,000 lb/hr of ammonia.

To perform the initial sizing, follow these steps:

1. Click the **Run All** button on the main CHEMCAD toolbar to calculate the flow information for streams 2 and 3. Both streams should be at -9° F, 225 psig, and 113,000 lb/hr of ammonia.
2. Click stream 2 to select it. The stream is selected when it is shown bracketed by black squares. Select **Sizing** > **Control Valve** to bring up the Control Valve Sizing dialog box.

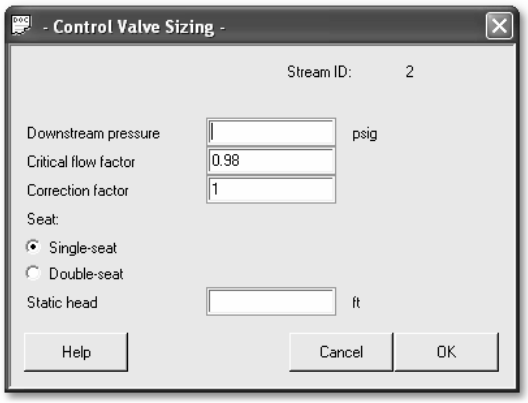


Figure 11-50: The Control Valve Sizing dialog box

3. In the **Downstream pressure** field, enter **15**. Click **OK** to display a control valve sizing report in a separate window. CHEMCAD reports the properties of the stream and the calculated parameters for the valve.
4. Repeat the procedure for stream 3, using a downstream pressure of 0.2 psig.

Rating Case

The next task is to rate these valves in a simulation. You need to determine the valve position for these valves in this service at 113,000 lb/hr. Since this task models the behavior of the control valves, you will need a slightly larger flowsheet, as shown in Figure 11-51.

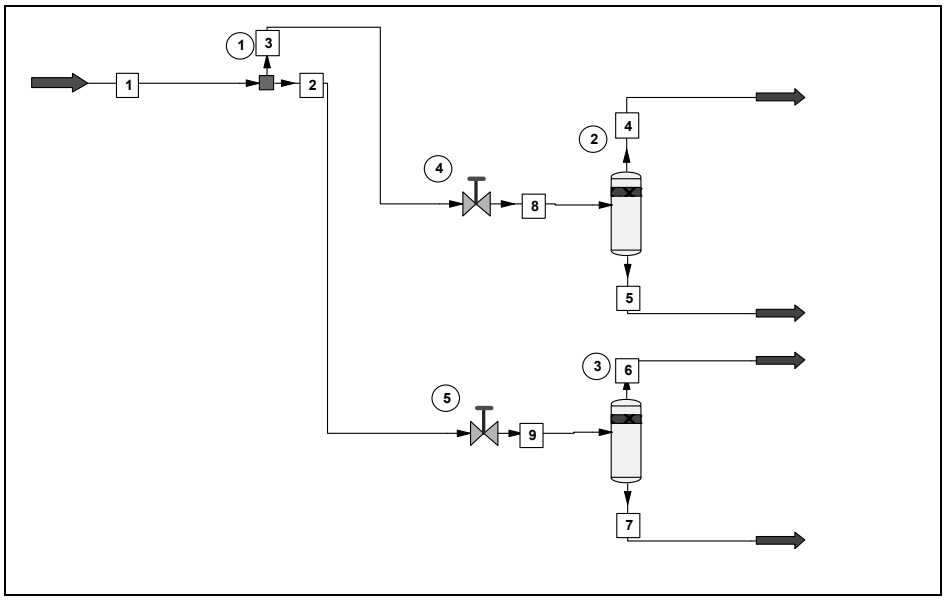


Figure 11-51: Flowsheet for rating valves in a simulation

The flash UnitOps at the end are not necessary; they are included to illustrate the vapor and liquid flow rates in separate streams if flashing occurs.

The divider is still set to 113,000 lb/hr, and the flash tanks are set to the mode called **Specify T and P; calculate V/F and Heat**. Flash UnitOp #2 is set to -1° F and 15 psig. Flash UnitOp #3 is set to -28° F and 0 .2 psig.

Follow these steps to rate the control valves:

1. Double-click the icon for control valve #4 to open the Control Valve dialog box.

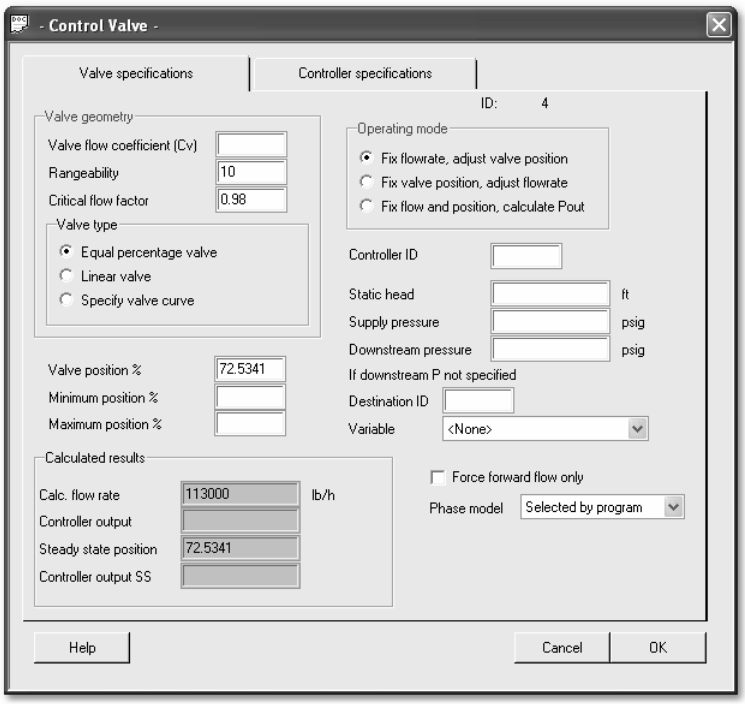


Figure 11-52: The Control Valve dialog box

2. In the **Valve flow coefficient (Cv)** field, enter **36**. In the **Downstream pressure** field, enter **15**. Select the **Operating mode** option called **Fix flowrate, adjust valve position**. Click **OK**.
3. Now double-click the icon for control valve #5. For this valve, select the same operating mode that you used for valve #4. Specify a valve flow coefficient of 54 and a downstream pressure of 0.2 psig, and then click **OK**.
4. Click the **Run All** button on the toolbar to run the simulation.
5. To view the results, first click a blank area of the CHEMCAD workspace to ensure that no UnitOps are currently selected. Then select **Report** > **UnitOps** > **Select UnitOps**.
6. In the Select UnitOps dialog box, type **4**, press **[RETURN]**, and then type **5**. Click **OK** to bring up a report for these two valves.

The report shows that valve #4 is at 72.5% open, and valve #5 is at 53.3% open.

To see how much vaporization occurs across valve #5, right-click the valve and select **View Stream Properties**. This volume change is why CHEMCAD chose a larger valve for the second stream. With the vaporization occurring in the valve, a smaller two-inch valve body would be approaching sonic velocity through the valve body.

Flow Rate as a Function of Pressure

In typical CHEMCAD simulations, information flows in one direction: downstream. Upstream conditions determine the downstream conditions. In most simulations, you simply set the flow rates and pressures of feed streams. Pressure drops are either calculated based on flow or specified through UnitOps, and the downstream pressures, flow rates, and so forth are calculated when you run the simulation.

For piping simulations, flow rate and pressure are dependent on each other. The backpressure on valves, pipes, and other UnitOps affects the flow rate through the valve. Likewise, the flow rate through a valve (or through a pipe or a pump) determines the downstream pressure.

In flow models like the control valve sizing model, it is sometimes useful to let flow rate vary as a function of the pressure. For example, suppose a process upset in the system shown in Figure 11-53 caused the pressure in vessel D-2 to rise from 15 psig to 30 psig. Assuming the upset occurs faster than the valves react, what is the new flow rate from D-1?

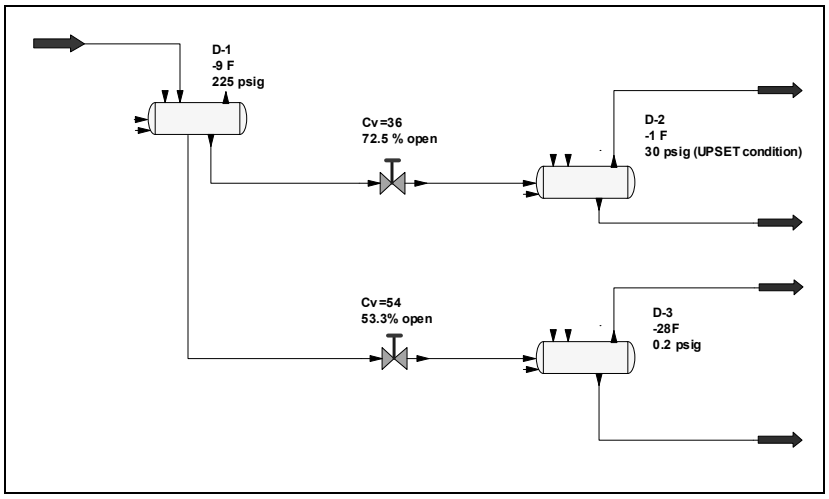


Figure 11-53: Vessel D-2 in an upset condition

To answer this question, you need a special UnitOp called a *node*. A node is a point in the simulation that has a pressure, a flow coming in, and a flow going out. The node units create a network, solving for flow rate at each point based on the fixed pressures. Nodes are placed on the flowsheet immediately upstream and downstream from each control valve. Figure 11-54 shows the system with nodes in place.

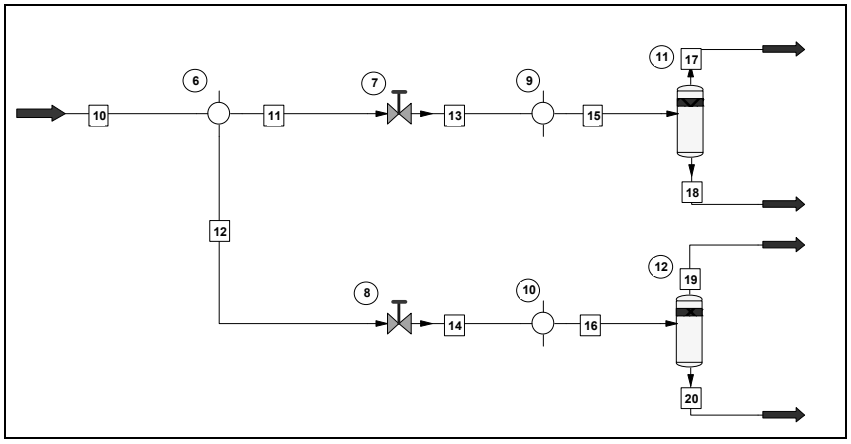


Figure 11-54: Nodes located upstream and downstream from control valves

The function of the divider—to split the incoming flow—is now handled by node #6. The node will balance the flow rates so that all streams entering and exiting the node are at the same pressure. Nodes are also placed between the flash vessels and the control valves. At the nodes you can fix the pressures, and let the flow rate vary as a function of valve position and pressure difference.

To see how these nodes are set up, you can double-click node #6 to open the Node dialog box.

Figure 11-55: The Node dialog box

The fixed pressure at this node is 225 psig. The inlet flow mode is set to **Free inlet stream**, and the two outlet streams are set to **Flow set by UnitOp**. The flow into each control valve will be determined by the control valve opening position and the pressure difference across the valve.

For node #9, the fixed pressure is set to 30 psig, and for node #10, the pressure is 0.2 psig. Flow into each of these nodes is controlled by the control valve using the **Flow set by UnitOp** mode; flow out is set to **Free Outlet stream**.

The control valves need to be changed to fix the valve position and calculate flow rate. To do this, set the **Operating mode** for each valve **to Fix valve position, adjust flowrate**.

After making this change, click the **Run All** toolbar button to run the simulation. After running, you can view the streams around node #6 by right-clicking the node and selecting **View stream composition**. The resulting report (Figure 11-56) shows that the flow rate for stream 11 (upstream from D-2) has dropped from 113,000 lb/hr to 109,138 lb/hr. This illustrates the effect of backpressure on the flow rates through the valves.

Job Name: Example1-Node Date: 10/19/2008 Time: 15:29:45

Stream No.	10	11	12
Stream Name			
Temp F	-9.0000*	-9.0000	-9.0000
Pres psig	225.0000*	225.0000	225.0000
Enth MMBtu/h	-399.52	-196.29	-203.23
Vapor mole fraction	0.00000	0.00000	0.00000
Total lbmol/h	13043.2031	6408.2427	6634.9609
Total lb/h	222139.0000	109138.7813	113000.0234
Total std L ft3/hr	5749.4379	2824.7504	2924.6877
Total std V scfh	4949617.00	2431791.00	2517825.75
Flowrates in lb/h			
Ammonia	222139.0000	109138.7813	113000.0234

Figure 11-56: Stream composition report for node #6

Simple Flow Example

This portion of the piping tutorial covers control valve sizing, feedback controllers, NPSH, orifice sizing/rating, pipe sizing/rating, and the Pipe UnitOp.

Problem Statement

The piping system shown must be designed to transport 120 gpm of glacial acetic acid at 70-140° F. The pressure at the inlet is known at 20 psia, and the outlet must be no less than 20 psia. The piping system and its individual elements must be sized for design conditions and then rated at operating conditions. The goal is to determine the $NPSH_a$ and head requirements for future pump selection.

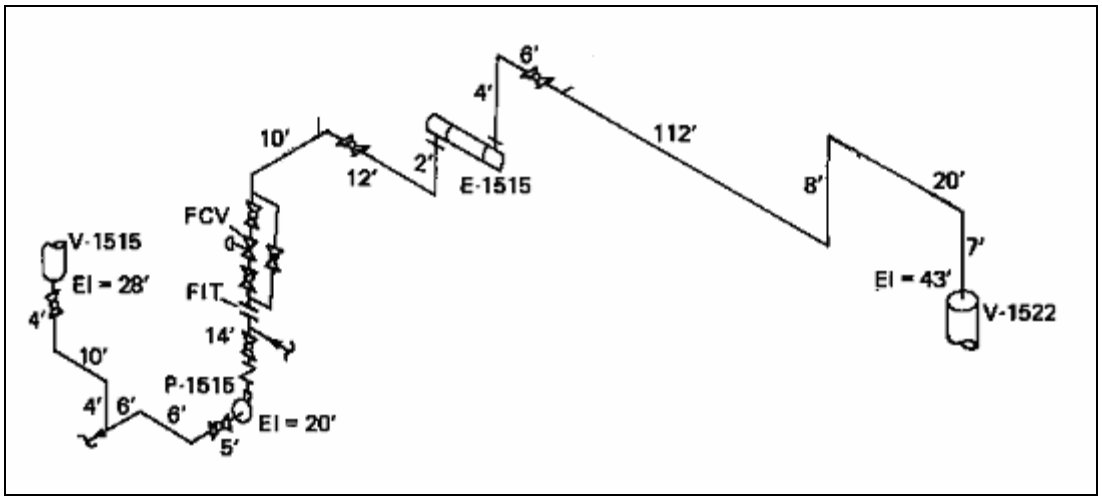


Figure 11-57: Piping isometric for this problem

This example is called **Example 2**, and it's located in the located in the **My Simulations\Examples\Piping** folder.

Creating the Simulation

Follow these steps to create and run this simulation:

1. Convert the piping isometric in Figure 11-57 to a CHEMCAD flowsheet. Pipe UnitOps are used to represent entire sections of piping, including fittings:
2. Select **Sizing** > **Piping** and select the applicable streams to bring up the Pipe Sizing dialog box.

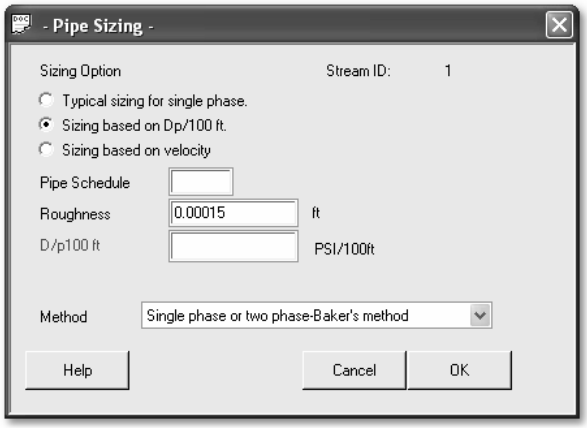


Figure 11-58: The Pipe Sizing dialog box

3. Select the **Typical sizing for single phase** option and use standard schedule 40 pipe. Click **OK** to view a line sizing report for the selected stream.

Note: Since the fluid in this system is sub-cooled liquid and all flows are constant, this calculated line size should apply to all piping in the system. The exception is the pump suction pipe, which as a general rule should be one size larger.

4. Select **Sizing** > **Orifice** and select the stream on the discharge side of the pump. In the Orifice Sizing dialog box, select **D and D/2** pressure taps, enter **3** as the pipe inside diameter, and enter **100** as the water differential pressure. Click **OK** to bring up an orifice sizing report for the selected stream.

Note: Using the calculated bore hole, CHEMCAD determines the flow resistance factor of the orifice as shown:

$$C = C_d / (\sqrt{(1 - \beta^4)})$$

$$Kr \approx \frac{1 - \beta^2}{C^2 \beta^4}$$

The orifice sizing report gives the Kr value, which you will use later in the Pipe Sizing and Rating dialog box.

5. To size the control valve, select stream #1 and then select **Sizing** > **Control Valve**. In the **Downstream pressure** field, enter **15**, and select the **Single-seat** option. Since stream #1 is at 20 psia, you are simply sizing a control valve to produce a pressure drop of 5 psi. Click **OK** to view a control valve sizing report for the selected stream.

6. Double-click control valve #4 to open the Control Valve dialog box. Enter the valve flow coefficient (Cv) of the valve from the sizing report, set the valve position to **50**%, and set the operating mode to **Fix flow and position, calculate Pout**. Click **OK** to save these settings and close the dialog box.

7. Double-click the heat exchanger icon to open the Simple Heat Exchanger dialog box. Enter a pressure drop of **2** psi and set the outlet temperature to **140**° F. Click **OK** to continue.
8. Tabulate and specify the valves, fittings, pipe lengths, and elevation changes of each section of pipe. For all of these pipes, set the **Method** field to **2 Single Phase flow**, set the **Sizing option** to **0 Rating**, and use flanged fittings throughout.

Pipe #1	**Pipe #3 (before control valve)**
1 entrance, well rounded	1 swing check valve, clearway
2 ball valves	2 ball valves
4 standard elbows, 90-degree	2 tee, flow-through run
1 tee, flow-through branch	1 orifice plate (as previously determined)
35 feet of piping	14 feet of piping
-8′ elevation change	14′ elevation change

Pipe #5 (after control valve)	**Pipe #7 (after E-1515)**
2 ball valves	1 ball valve
2 tee, flow-through run	4 standard elbows, 90-degree
3 standard elbows, 90-degree	1 tee, flow-through run
1 exit from pipe	1 well rounded entrance
24 feet of piping	1 exit from pipe
2′ foot elevation change	157 feet of piping
	5′ elevation change

9. Specify the pump outlet pressure at some arbitrary value (try 25 psia) and make a trial run. Check the calculated outlet pressure. You can then iterate to find the required pump head.

Using Controllers to Simplify the Problem

While manually changing the pump outlet pressure will get you where you need to be, it's easier to let CHEMCAD do the work. The Controller UnitOp can adjust this pressure for you.

A feedback controller in CHEMCAD has nothing to do with process control valves or PID settings. In a CHEMCAD steady-state model, the term *feedback control* refers to a mathematical controller. It's a math tool used to adjust a variable on a flowsheet until a target value reaches a specified value.

Follow these steps to use a feedback controller to calculate the required outlet pressure:

1. Right-click stream #8 and select **Insert unit**. Click **OK** at the pop-up message and then click the **Controller** tool in the All UnitOps palette.
2. Click near the existing stream to place a controller icon on the flowsheet. The stream automatically re-routes through this icon, as shown in Figure 11-59.

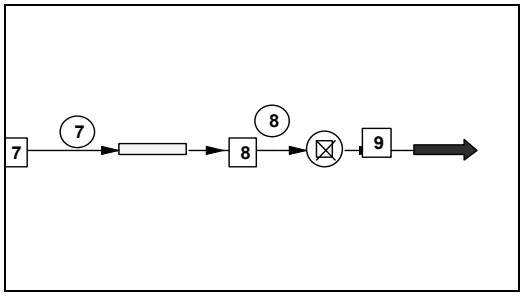


Figure 11-59: Insertion of feedback controller

3. In the Controller dialog box, specify the following and then click **OK**:
   - *Controller mode:* **Feed-backward**
   - *Adjust this variable:* **Unitop**, ID number **2**, Variable **2 Output pressure**
   - *Until this:* **Stream**, ID number **8**, Variable **2 Pressure**
   - *Is equal to this target:* Constant **20**, Units **4 Pressure**

When you run the simulation, the controller will automatically change the pump outlet pressure until the pressure leaving the last pipe unit is equal to 20 psia. You now know the head requirements for your pump.

Calculating NPSHA

The net positive suction head, better known as NPSH, is defined as the total pressure available at the pump suction minus the pumping fluid's vapor pressure. It is almost always reported in feet of pumped fluid or water.

Every pump has a specified NPSH requirement (*NPSHr*) at a given operating speed. To ensure reliable operation, the available NPSH (*NPSHa)* must be greater than the NPSHr. If not, cavitation and shortened service life may result.

To select the appropriate pump, you need to calculate NPSHa. In CHEMCAD, this is an easy task. Simply check the **Calculate NPSHa** box in the Pump dialog box, and then run the simulation. Now when you pull up the Pump dialog box, the calculated NPSHa is displayed.

Note: It is important to the NPSHa calculation that the inlet piping to the pump be correctly specified. If the piping specifications are not complete, the pressure at the inlet may not be accurate, leading to an inaccurate NPSHa calculation

Branched Flow Example

This portion of the piping tutorial covers the Node UnitOp, pipe networks, pump selection criteria, and Pump UnitOp performance curves.

Problem Statement

The previous piping system has been changed. Due to the branched flow to the two heat exchangers, the problem is no longer a simple one.

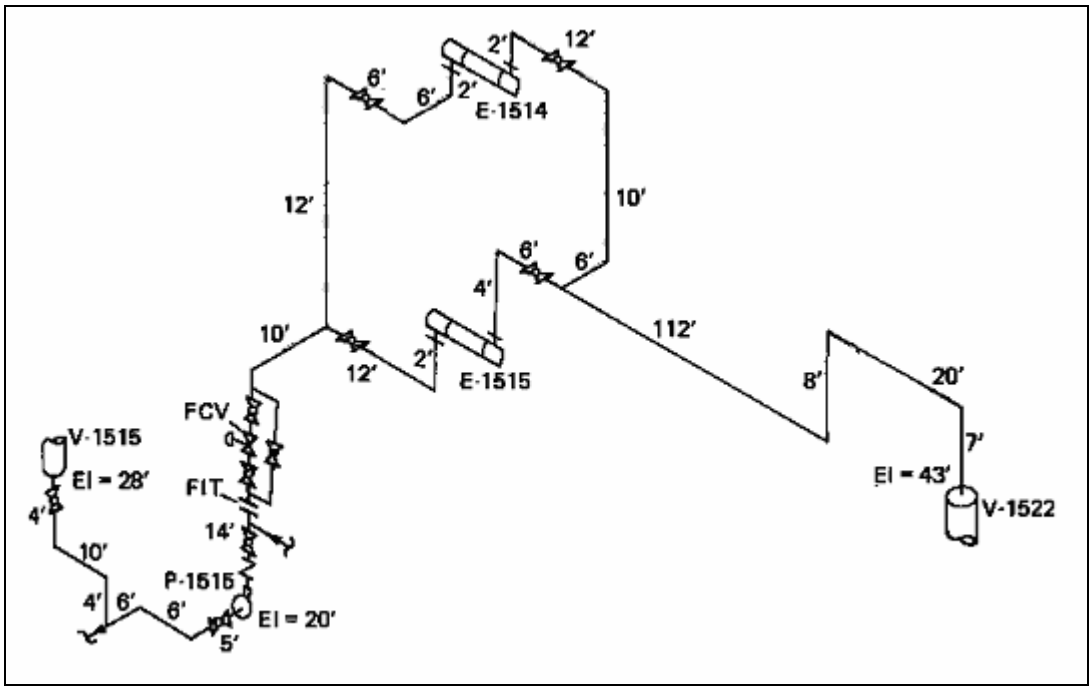


Figure 11-60: Piping isometric showing branched flow

This example is called **Example 3**, and it's located in the located in the **My Simulations\Examples\Piping** folder.

The branched flow is a difficult problem to solve using the controller approach. Both exchangers have different piping and therefore different flow rates. You need an approach where you split and recombine flows, and have the simulation calculate the pressure and flow rates in an iterative manner. The Node UnitOp gives you this flexibility.

Remember that a node is a point where pressure is uniform. There may be multiple inlets and outlets. The flow rates for each stream will be balanced by CHEMCAD to reach a single pressure. You can specify the pressure or allow it to vary.

Creating the Simulation

Convert the piping isometric to a CHEMCAD flowsheet, as shown in Figure 11-61.

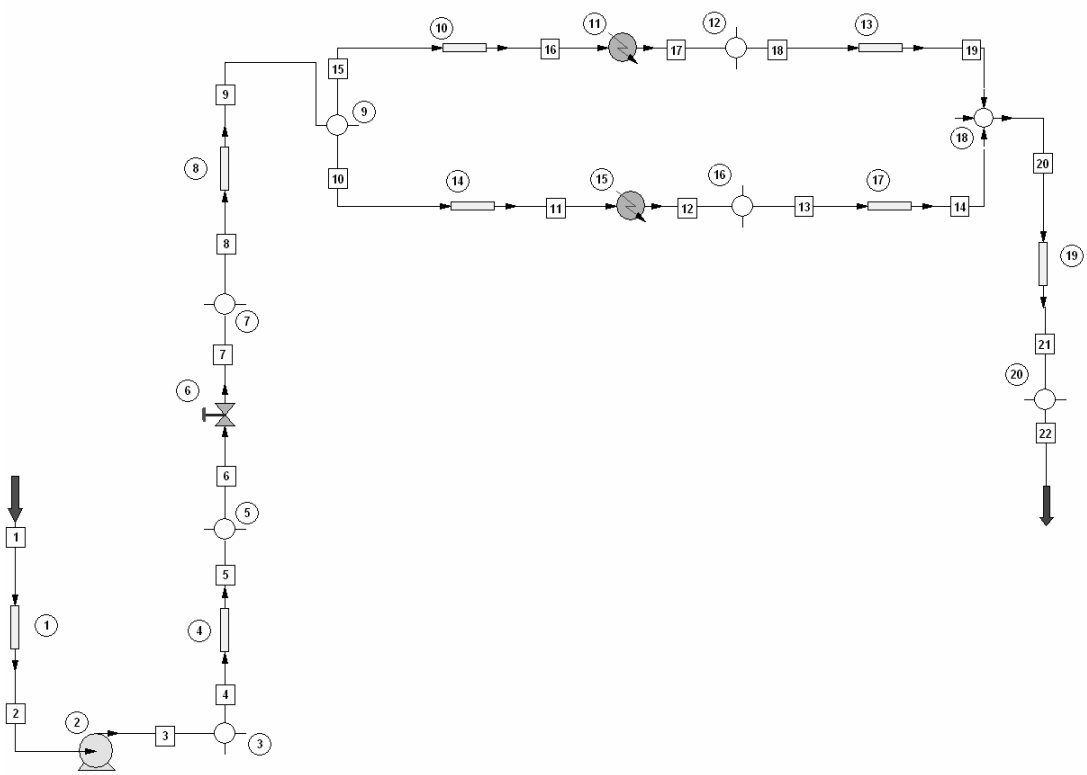


Figure 11-61: The flowsheet representing this piping system

In CHEMCAD, Pipe UnitOps are used to represent entire sections of piping, including fittings. Node UnitOps are placed where pressure or flow rate are unknown.

For this example, assume a pressure drop of 2 psi across each heat exchanger. Tabulate the valves, fittings, pipe lengths, and elevation changes of each section of pipe. Use flanged fittings throughout.

Pipe #1	**Pipe #2 (before control valve)**
1 entrance, well rounded	1 swing check valve, clearway
2 ball valves	2 ball valves
4 standard elbows, 90-degree	2 tee, flow through run
1 tee, flow through branch	1 orifice plate (as determined above)
35 feet of piping	14 feet of piping

Pipe #3 (after control valve)	**Pipe #4 (to E-1514)**
1 ball valve	1 tee, flow through branch
1 tee, flow through run	1 ball valve
2 standard elbows, 90-degree	1 exit from pipe
10 feet of piping	3 standard elbows, 90-degree
	26 feet of piping

Pipe #5 (from E-1514)	Pipe #6 (to E-1515)
1 ball valve	1 ball valve
1 well rounded entrance	1 exit from pipe
3 standard elbows, 90-degree	1 tee, flow-through run
1 tee, flow-through branch	1 standard elbows, 90-degree
30 feet of piping	14 feet of piping

Pipe #7 (from E-1515)	Pipe #8 (to V-1522)
1 standard elbow, 90-degree	3 standard elbows, 90-degree
1 ball valve	1 exit from pipe
1 well rounded entrance	147 feet of piping
1 tee, flow-through run	
10 feet of piping	

At this time you don't know the pump specifications, so set the pump to **Specify Outlet Pressure** and leave the pressure specification blank. The Node UnitOp will solve for the pressure increase, and set the pump outlet pressure accordingly.

Set up the nodes with the following information:

- **Node 3:** Variable pressure, use current stream rate for inlet, flow set by UnitOp for outlet, elevation = 20 feet
- **Node 5:** Variable pressure, flow set by UnitOp for both inlet and outlet, elevation = 34 feet
- **Node 7:** Variable pressure, flow set by UnitOp for both inlet and outlet, elevation = 34 feet
- **Node 9:** Variable pressure, flow set by UnitOp for both inlet and outlet, elevation = 34 feet
- **Node 12:** Variable pressure, flow set by UnitOp for both inlet and outlet, elevation = 50 feet
- **Node 16:** Variable pressure, flow set by UnitOp for both inlet and outlet, elevation = 38 feet
- **Node 18:** Variable pressure, flow set by UnitOp for both inlet and outlet, elevation = 42 feet
- **Node 20 (last node):** Fixed pressure, 20 psia, flow set by UnitOp for inlet, free outlet stream for outlet, elevation = 43 feet

Running the Simulation

To run the simulation, click the **Run All** button on the main CHEMCAD toolbar.

Once the simulation has run, check the Pump UnitOp's pressure increase. This tells you the head requirements of the pump. Using this information and the flow rate (120 gpm), you can consult a pump handbook to determine the correct pump size.

Selecting a Pump

The following pump curve data is representative of the type of equipment that would be appropriate for this application.

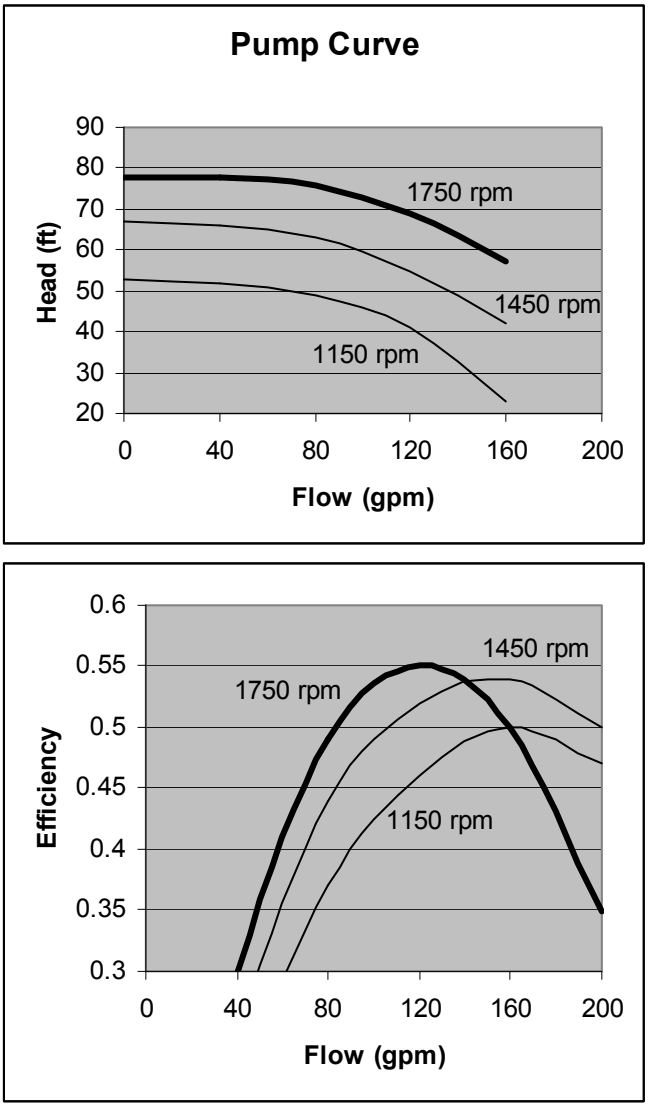


Figure 11-62: Combined pump curves for a sample pump

To enter this curve into your pump, open the Pump dialog box and select **Specify Performance Curve** for the pump mode. This setting allows you to enter multiple speed lines and an operating speed. For the purposes of this tutorial, enter 1 for the number of speed lines and set the pump speed to **1750** RPM. Click **OK** to bring up the Performance Curve dialog box.

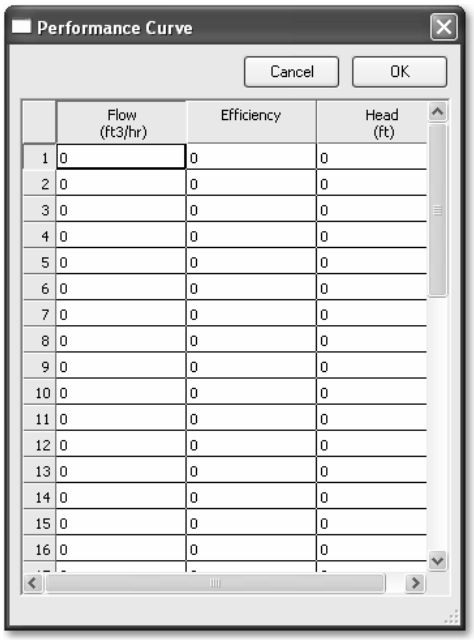


Figure 11-63: The Performance Curve dialog box

Here you can enter as many points as you want to define your curve. CHEMCAD will fit a quadratic equation to the points, creating a smooth curve fit for your data.

Now that you have entered the pump performance curve, you must add node UnitOps to the suction side of the pump to allow the flow rate to vary. In this way, you can calculate the maximum flow rate of your system.

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